Quantum Mechanics Problems

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Introduction

Quantum Mechanics Problems (QMP) is a source book for instructors of introductory quantum mechanics. The book is available in electronic form to instructors by request to the author. It is free courseware and can be freely used and distributed, but not used for commercial purposes. The aim of QMP is to provide digestable problems for quizzes, assignments, and tests for modern students. There is a bit of spoon-finding—nourishing spoon-feeding I hope.

The problems are grouped by topics in chapters: see Contents below. The chapter ordering follows roughly the traditional chapter/topic ordering in quantum mechanics textbooks. For each chapter there are two classes of problems: in order of appearance in a chapter they are: (1) multiple-choice problems and (2) full-answer problems. Almost all the problems have complete suggested answers. The answers may be the greatest benefit of QMP. The questions and answers can be posted on the web in pdf format.

The problems have been suggested by many sources, but have all been written by me. Given that the ideas for problems are the common coin of the realm, I prefer to call my versions of the problems redactions. Instructors, however, might well wish to find solutions to particular problems from well known texts. Therefore, I give the suggesting source (when there is one and I recall what it was) by a reference code on the extra keyword line: e.g., (Gr-10:1.1) stands for Griffiths, p. 10, problem 1.1. Caveat: my redaction and the suggesting source problem will not in general correspond perfectly or even closely in some cases. The references for the source texts and other references follow the contents. A general citation is usually, e.g., Ar-400 for Arfken, p. 400.

At the end of the book are three appendices. The first is set of review problems anent matrices and determinants. The second is an equation sheet suitable to give to students as a test aid and a review sheet. The third is a set of answer tables for multiple choice questions.

Quantum Mechanics Problems is a book in progress. There are gaps in the coverage and the ordering of the problems by chapters is not yet final. User instructors can, of course, add and modify as they list.

Everything is written in plain TeX in my own idiosyncratic style. The questions are all have codes and keywords for easy selection electronically or by hand. A fortran program for selecting the problems and outputting them in quiz, assignment, and test formats is also available. Note the quiz, etc. creation procedure is a bit klutzy, but it works. User instructors could easily construct their own programs for problem selection.

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Appendices

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Chapt. 1 Classical Physics in Trouble

Multiple-Choice Problems

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001 qmult 00100 1 1 3 easy memory: quantum mechanics

1. The physical theory that deals mainly with microscopic phenomena is:

   a) quartz mechanics.
   b) quarks mechanics.
   c) quantum mechanics.
   d) quantum jump mechanics.
   e) quasi-mechanics.

---

001 qmult 00200 1 1 1 easy memory: photon energy

2. The photon, the quantum of electromagnetic radiation, has **ENERGY**:

   a) $hf = \hbar\omega$.
   b) h/λ.
   c) $\hbar k$.
   d) $h^2 f$.
   e) hf^2.

---

001 qmult 00300 1 1 4 easy memory: photoelectric effect

3. A key piece of evidence for the wave-particle duality of light is:

   a) the photograph effect.
   b) the Maxwell's electrodynamics as summarized in the four Maxwell's equations.
   c) the frequency of red light.
   d) the photoelectric effect.
   e) the photomagnetic effect.

---

001 qmult 00400 1 1 1 easy memory: Compton effect

4. Einstein predicted and Compton proved that photons:

   a) have linear momentum.
   b) do not have linear momentum.
   c) sometimes have linear momentum.
   d) both have and do not have linear momentum at the same time.
   e) neither have nor have not linear momentum.

---

001 qmult 00500 1 4 3 easy deducto-memory: Bohr atom

5. "Let's play *Jeopardy*! For \$100, the answer is: This model of an atom is of historical and pedagogical interest, but it is of little use in modern practical calculations and from the modern standpoint is probably misleading rather than insight-giving."

   What is ____________, Alex?

a) Schrödinger's model of the hydrogen atom
b) the Thomas-Fermi model of a many electron atom
c) Bohr's model of the hydrogen atom d) the liquid drop model of the atom
e) the model hydrogen atom of Leucippos and Democritos

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001 qmult 00550 1 1 4 easy memory: hydrogenic energy formula

6. The formula

$$E_n = -\frac{1}{2} m_e c^2 \alpha^2 \frac{Z^2}{n^2}$$

gives the main energy levels of:

a) positronium.
b) magnesium deboride.
c) the hydrogen molecule.
d) the hydrogenic atom.
e) the infinite square well.

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001 qmult 00600 1 1 5 easy memory: Greek atomists

7. The atomic theory was first proposed by the ancient Greeks Leucippos (5th century BCE) and Democritos (5th to 4th century BCE: he reputedly lived to be 100). The term atomos means uncut: e.g., the grass is atomos. The atomists started from a philosophical position that there had to be something to give stability to nature: obviously the macroscopic world was full of change: therefore what was imperishable or uncutable—atoms—must be below perception. The modern quantum theory does indeed bear out some of their thinking. Microscopic particles can be created and destroyed, of course, but the members of a class are much more identical than macroscopic objects can ever be: fundamental particles like electrons and quarks are thought to be absolutely identical. Thus the forms particles can take are apparently eternal: a hydrogen atom today is the same in theory as one at any time in universal history.

The atomists tried to work out an atomic understanding of existence in general. For instance they constructed a cosmology using atoms that bears some resemblance to modern eternal inflationary cosmology in which there are infinitely many universes that are born out of primordial space-time foam and perhaps return to that—foam to foam. Unfortunately, the atomists got off on the wrong foot on the shape of the Earth: they were still flat Earthers when the round Earth theory was being established. Quite obviously to us, the atomists were badly non-experimental. Much of their thinking can be called rational myth. To a degree they were lucky in happening to be attracted to an essentially right idea.

The atomists were eventually stigmatized as atheists: they did not deny that gods exist, but didn't leave anything for the gods to do. This may have been their downfall. The more orthodox and popular philosophies of Plato, Aristotle, and the Stoics rejected atomism probably, among other things, for its seeming atheism. Christianity followed suit in this regard. The writings of the atomists only exist in fragments—and Democritos seems to have been as famous as Plato in his day. The Epicurean philosophers adopted atomism, but also suffered the stigmatization as atheists—and also hedonists who are, of course, the worst. But the atom idea lingered on through the centuries: Leucippos and Democritos, Epicurus, Lucretius (his surviving poem *De Rerum Natura* [*On Nature*] expounds atomism), Gassendi (17th century), Newton, Dalton: the chain is unbroken: it is not true that modern atomism has no historical or essential connection to ancient atomism.

A good account of ancient atomism can be found in David Furley's *The Greek Cosmologists*.

Now, without recurring to the top of this preamble, atomism was invented in:

a) the early 19th century. b) the 17th century by Gassendi.
c) the 10th century CE. d) the 5th century CE. e) the 5th century BCE.

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001 qmult 00800 1 1 1 easy memory: causality, relativity

8. Einstein ruled out faster than light signaling because:

   a) it would cause irresolvable causality paradoxes.
   b) it would not cause irresolvable causality paradoxes.
   c) it led to irresolvable paradoxes in quantum mechanics.
   d) it would destroy the universe.
   e) it had been experimentally verified.

---

001 qmult 00900 1 1 3 easy memory: EPR paradox

9. The Einstein-Podolsky-Rosen (EPR) paradox was proposed to show that ordinary quantum mechanics implied superluminal signaling and therefore was:

   a) more or less correct.
   b) absolutely correct.
   c) defective.
   d) wrong in all its predictions.
   e) never wrong in its predictions.

---

001 qmult 01000 1 4 3 easy deducto-memory: Bell's theorem

10. "Let's play *Jeopardy*! For \$100, the answer is: This theorem (if it is indeed inescapably correct) and the subsequent experiments on the effect the theorem dealt with show that quantum mechanical signaling exceeds the speed of light."

    a) What is Dark's theorem, Alex?
    b) What is Midnight's theorem, Alex?
    c) What is Bell's theorem, Alex?
    d) What is Book's theorem, Alex?
    e) What is Candle's theorem, Alex?

Full-Answer Problems

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001 qfull 00500 3 5 0 tough thinking: Rutherford's nucleus

Extra keywords: (HRW-977:62P)

1. Rutherford discovered the nucleus in 1911 by bombarding metal foils with alpha particles now known to be helium nuclei (atomic mass 4.0026). An alpha particle has positive charge $2e$. He expected the alpha particles to pass right through the foils with only small deviations. Most did, but some scattered off a very large angles. Using a classical particle picture of the alpha particles and the entities they were scattering off of he came to the conclusion that atoms contained most of their mass and positive charge inside a region with a size scale of $\sim 10^{-15}\,\mathrm{m} = 1\,\mathrm{fm}$: this 10^{-5} times smaller than the atomic size. (Note fm stands officially for femtometer, but physicists call this unit a fermi.) Rutherford concluded that there must be a dense little core to an atom: the nucleus.

   a) Why did the alpha particles scatter off the nucleus, but not off the electrons? **HINTS:** Think dense core and diffuse cloud. What is the force causing the scattering?

   b) If the alpha particles have kinetic energy 7.5 Mev, what is their de Broglie wavelength?

   c) The closest approach of the alpha particles to the nucleus was of order 30 fm. Would the wave nature of the alpha particles have had any effect? Note the wave-particle duality was not even suspected for massive particles in 1911.

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001 qfull 01000 3 5 0 tough thinking: black-body radiation, Wien law

Extra keywords: (Le-62) gives a sketch of the derivations

2. Black-body radiation posed a considerable challenge to classical physics which it was partially able to meet. Let's see how far we can get from a classical, or at least semi-classical, thermodynamic equilibrium analysis.

   a) Let U_λ be the radiation energy density per wavelength of a thermodynamic equilibrium radiation field trapped in some kind of cavity. The adjective thermodynamic equilibrium implies that the field is homogenous and isotropic. I think Hohlraum was the traditional name for such a cavity. Let's call the field a photon gas and be done with it—anachronism be darned. Since the radiation field is isotropic, the specific intensity is then given by

   $$B(\lambda,T)=\frac{cU_\lambda}{4\pi}\ , \tag{Pr.1}$$

   where c is of course the speed of light. Specific intensity is radiation flux per wavelength per solid angle. From special relativity (although there may be some legitimately classical way of getting it), the momentum flux associated with a specific intensity is just $B(\lambda,T)/c$. Recall the rest plus kinetic energy of a particle is given by

   $$E=\sqrt{p^2c^2+m_0^2c^4}\ , \tag{Pr.2}$$

   where p is momentum and m_0 is rest mass. From an integral find the expression for the radiation pressure on a specularly reflecting surface:

   $$p=\frac{1}{3}U\ , \tag{Pr.3}$$

   where p is now pressure and U is the wavelength-integrated radiation density. Argue that the same pressure applies even if the surface is only partially reflecting or pure blackbody provided the the radiation field and the surface are in thermodynamic equilibrium. **HINT:** Remember to account for angle of incidence and reflection.

   b) Now we can utilize a few classical thermodynamic results to show that

   $$U=aT^4\ , \tag{Pr.4}$$

   where a is a radiation constant related to the Stefan-Boltzmann constant $\sigma=5.67051\times 10^5\,\mathrm{ergs/(cm^2\,K^4)}$ and T is Kelvin temperature, of course. The relation between a and σ follows from the find the flux leaking out a small hole in the Hohlraum:

   $$F=2\pi\int_0^1\frac{cU}{4\pi}\mu\,d\mu=\frac{ca}{4}T^4\ , \tag{$Pr.5$}$$

   where μ is the cosine of the angle to the normal of the surface where the hole is. One sees that $\sigma=ca/4$. Classically a cannot be calculated theoretically; in quantum mechanical statistical mechanics a can be derived. The proportionality $U\propto T^4$ can, however, be derived classically. Recall the 1st law of thermodynamics:

   $$dE=T\,dS-p\,dV\ , \tag{Pr.6}$$

   where E is internal energy, S is entropy, and V is volume. Note that

   $$\left(\frac{\partial E}{\partial S}\right)_V=T\qquad\text{and}\qquad\left(\frac{\partial E}{\partial V}\right)_S=-p\ , \tag{Pr.7}$$

where the subscripts indicate the variables held constant. It follows from calculus (assuming well-behaved functions) that

$$\left(\frac{\partial p}{\partial S}\right)_V = -\left(\frac{\partial T}{\partial V}\right)_S , \tag{Pr.8}$$

The last relation is one of Maxwell's four thermodynamic relations—Newton did things in threes; Maxwell in fours. Note that $E = UV$ for a radiation field. Now go to it: show $U \propto T^4$.

c) As a by-product of the part (b) answer, you should have found that

$$T \propto V^{-1/3} \tag{Pr.9}$$

for a quasistatic adiabatic process with the photon gas. (Find it now if somehow you missed it in the part (b) answer.) Assume you have a perfectly reflecting Hohlraum that you expand homologously by a scaling factor $f(t)$, where t is time. Thus at any time t any length ℓ between physical points on the walls in the system is given by

$$\ell = f(t)\ell_0 , \tag{Pr.10}$$

where ℓ_0 was the physical length at t_0 when $f(t_0) = 1$. Find out how T, U, $U\,dV$, and E scale with $f(t)$. What happens to the lost internal energy? **HINT:** This is easy.

d) Consider the process described in the part (c) and show that

$$\lambda = \lambda_0 f(t) \tag{Pr.11}$$

for each specific intensity beam. Note you can use the non-relativistic Doppler effect since the velocity shift between scatterings off the walls is vanishingly small in the quasistatic limit.

e) For the same system as in part (c) show that

$$B(\lambda, T)\, d\lambda\, dV = f(t)^{-1} B(\lambda_0, T_0)\, d\lambda_0\, dV_0 . \tag{Pr.12}$$

Then show that equation (Pr.12) leads naturally (if not absolutely necessarily so far as I can see) to the prescription for black-body specific intensity

$$B(\lambda, T) = \lambda^{-5} g(x) = \left(\frac{T}{x}\right)^5 g(x) , \tag{Pr.13}$$

where

$$x \equiv \lambda T \tag{Pr.14}$$

and $g(x)$ is a universal function that cannot be determined from classical theory. Equation (Pr.13) is sometimes called Wien's displacement law. However the name Wien's displacement law is more usually (I think) reserved for the immediate result that for fixed T the the maximum of the black-body specific intensity (i.e., the maximum of $x^{-5}g(x)$) occurs at a wavelength given by

$$\lambda = \frac{x_{\rm max}}{T} , \tag{Pr.15}$$

where $x_{\rm max}$ is the global universal location of maximum for the universal function $g(x)$. It was empirically known that black-body radiation had only one maximum with wavelength, and so this corresponds to $x_{\rm max}$. I think classically $x_{\rm max}$ has to be determined empirically.

Wien's radiation law was I believe a fit to the observations of Wien's displacement law. This law is

$$B(\lambda, T) = k_1 \left(\frac{T}{x}\right)^5 \exp\left(-\frac{k_2}{x}\right) , \tag{Pr.16}$$

where k_1 and k_2 had to be determined from the fit. Wien's law works well for short wavelengths ($x \lesssim x_{\rm max}$), but gives a poorish fit to the long wavelengths ($x \gtrsim x_{\rm max}$) (Pa-190, but note the x there is the inverse of the x here aside from a constant). The Rayleigh-Jeans law derived from a rather different classical starting picture gave a good fit to long wavelengths ($x >> x_{\rm max}$), but failed badly at shorter wavelengths (Pa-190, but note the x there is the inverse of the x here aside from a constant). In fact the Rayleigh-Jeans law goes to inifinity as x goes to zero and the total energy in a Rayleigh-Jeans radiation field is infinite (Le-64): this is sometimes called the ultraviolet catastrophe (BFG-106). The correct black-body specific intensity law was derived from a primitive quantum theory by Max Planck in 1900 (BFG-106). Planck obtained an empirically excellent fit to the black-body specific intensity and then was able to derive it from his quantum hypothesis. The Rayleigh-Jeans and Planck laws are the subject for another question.

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001 qfull 01100 2 5 0 moderate thinking: Bohr atom

3. In 1913, Niels Bohr presented his model of the hydrogen atom which was quickly generalized to the hydrogenic atom (i.e., the one-electron atom of any nuclear charge Z). This model correctly gives the main hydrogenic atom energy levels and consists of a mixture of quantum mechanical and classical ideas. It is historically important for showing that quantization is somehow important in atomic structure and pedagogically it is of interest since it shows how simple theorizing can be done. But the model is, in fact, incorrect and from the modern perspective probably even misleading about the quantum mechanical nature of the atom. It is partially an accident of nature that it exists to be found. Only partially an accident since it does contain correct ingredients.

And it is no accident that Bohr found it. Bohr knew what he wanted: a model that would successfully predict the hydrogen atom spectrum which is a line spectrum showing emission at fixed frequencies. He knew from Einstein's photoelectric effect theory that electromagnetic radiation energy was quantized in amounts $h\nu$ where $h = 6.62606896(33) \times 10^{-27}\,{\rm erg\,s}$ was Planck's constant (which was introduced along with the quantization notion to explain black-body radiation in 1900) and ν was frequency of the quantum of radiation. He recognized that Planck's constant had units of angular momentum. He knew from Rutherford's nuclear model of the atom that the positive charge of an atom was concentrated in region that was much smaller than the atom size and that almost all the mass of the atom was in the nucleus. He knew that there were negative electrons in atoms and they were much less massive than the nucleus. He knew the structure of atoms was stable somehow. By a judicious mixture of classical electromagnetism, classical dynamics, and quantum ideas he found his model. A more sophisticated mixture of these concepts would lead to modern quantum mechanics.

Let's see if we can follow the steps of the ideal Bohr—not the Bohr of history.

NOTE: This a semi-classical question: Bohr, ideal or otherwise, knew nothing of the Schrödinger equation in 1913. Also note that this question uses Gaussian CGS units not MKS units. The most relevant distinction is that electric charge

$$e_{\rm CGS} = \frac{e_{\rm MKS}}{\sqrt{4\pi\epsilon_0}}$$

which implies the fine structure constant in CGS is

$$\alpha = \frac{e^2}{\hbar c} \ .$$

Astronomy is all Gaussian CGS by the way.

a) Bohr thought to build the electron system about the nucleus based on the electrostatic inverse square law with the electron system supported against collapse onto the nucleus by angular momentum. The nucleus was known to be much tinnier than the electron system which gives the atom its volume. The nucleus could thus be a considered an immobile point center of force at the origin of the relative nucleus-electron coordinate system frame. This frame is non-inertial, but classically can be given an inertial-frame treatment if the electron is given a reduced mass given by

$$m = \frac{m_e m_{\rm nucleus}}{m_e + m_{\rm nucleus}} \approx m_e \left(1 - \frac{m_e}{m_{\rm nucleus}}\right) ,$$

where m_e the electron mass and $m_{\rm nucleus}$ is the nucleus mass. The approximation is valid for $m_e/m_{\rm nucleus} << 1$ which is true of hydrogen and most hydrogenic systems, but not, for example, for positronium (a bound electron and positron).
The electron—there is only one in a hydrogenic atom—was taken to be in orbit about the nucleus. Circular orbits seemed the simplest way to proceed. The electrostatic force law (in Gaussian cgs units) in scalar form for a circular orbit is

$$\vec{F} = -\frac{Ze^2}{r^2}\hat{r} ,$$

where Ze is the nuclear charge, e is the electron charge, and r is the radial distance to the electron, and $\hat{r}$ is a unit vector in the radial direction.

What is the potential energy of the electron with the zero of potential energy for the electron at infinity as usual? **HINT:** If the result isn't obvious, you can get it using the work-potential energy formula:

$$V = -\int \vec{F} \cdot d\vec{r} + \text{constant} .$$

b) Using the centripetal force law (which is really $F = ma$ for uniform circular motion)

$$\vec{F} = -\frac{mv^2}{r}\hat{r} ,$$

find an expression for the classical kinetic energy T of the electron in terms of Z, e, and r alone.

c) What is the total energy of the electron in the orbit?

d) Classically an accelerating charge radiates. This seemed well established experimentally in Bohr's time. But an orbiting electron is accelerating, and so should lose energy continuously until it collapses into the nucleus: this catastrophe obviously doesn't happen. Electrons do not collapse into the nucleus. Also they radiate only at fixed frequencies which means fixed quantum energies by Einstein's photoelectric effect theory. So Bohr postulated that the electron could only be in certain orbits which he called stationary states and that the electron in a stationary state did not radiate. Only on transitions between stationary states (sometimes called quantum jumps or leaps) was there an emission of radiation in a quantum of radiation or (to use an anachronism) a photon. To get the fixed energies of emission only certain energies were allowed for the stationary states. But the emitted photons didn't come out with equally spaced energies: ergo the orbits couldn't be equally spaced in energy. From the fact that Planck's constant h has units of angular momentum, Bohr hypothesized the orbits were quantized in equally spaced amounts of angular momentum. But h was not the spacing that worked. Probably after a bit of fooling around, Bohr found that $h/(2\pi)$ or, as we now write it, $\hbar$ was the spacing that gave the right answer. The allowed angular momenta were given by

$$L = n\hbar ,$$

where n is any positive non-zero integer. The n is now called the principal quantum number, but its meanings in the Bohr model and in modern quantum mechanics are somewhat different. The principal quantum number n determines the main spacing of the hydrogenic energy levels.

Rewrite kinetic energy T in terms of $n\hbar$ and solve for an expression for r in terms n, $\hbar$, Ze^2, and m only. **HINT:** Recall the classical expression for angular momentum of particle in a circular orbit is $L = mrv$.

e) Using the formula for r from the part (d) answer write an expression for the energy of a stationary state in terms of m, c, α, Z, and n only. The c is the speed of light and the α is the fine structure constant: recall that in Gaussian cgs units

$$\alpha = \frac{e^2}{\hbar c} \ .$$

This formula for orbit energy turns out to be correct for the spacing of the main energy levels. But these energyxhell doesn't, in fact, have angular momentum $n\hbar$: it consists of has orbitals (as we now call them) with angular momenta in the range $[0, n-1]$ in units of $\hbar$ (e.g., Gr-139).

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001 qfull 01300 2 3 0 moderate math: Compton scattering

Extra keywords: (Ha-323:1.1)

4. In 1916, Einstein proposed that photons carry momentum according to the following formula:

$$p = \frac{h}{\lambda} \ ,$$

where h is Planck's constant and λ is the photon wavelength (HRW-959). In 1924, Louis de Broglie applied the formula in inverse form to give a wavelength for massive particles: i.e.,

$$\lambda = \frac{h}{p}$$

which is called the de Broglie wavelength formula. In 1923, Arthur Compton carried out experiments with X-rays scattering off electrons which showed that Einstein's formula correctly accounted for the wavelength shift on scattering. The Compton shift formula is

$$\Delta\lambda = \lambda_{\rm C}(1 - \cos\theta) \ ,$$

where $\lambda_{\rm C} = h/(m_e c) = 0.02426$ Å is the Compton wavelength (with m_e being the electron mass) and θ is the scattering angle (i.e., the angle between incident and scattering directions). This formula can be derived from Einstein's formula using a relativistic particle collisional picture.

a) Assuming an electron starts at rest and is hit head-on by a photon "particle and the collision is elastic," what conservation law expressions can be used to relate incoming photon momentum p_1, outgoing photon momentum p_2, outgoing electron momentum p_e, photon scattering angle θ, and electron scattering angle ϕ? Can one solve for the four outgoing quantities given the initial conditions? **HINT:** Recall that the relativistic kinetic energy of a particle is given by

$$T = \sqrt{(pc)^2 + (m_0c^2)^2} - m_0c^2 = (\gamma - 1)m_0c^2 \ ,$$

where p is momentum and m_0 is the rest mass.

b) Solve for p_2 in terms of p_1 and θ only.

c) Now using Einstein wavelength formula, find Compton's formula.

d) Sketch the behavior of $\Delta\lambda$ as a function of θ. What is the shift formula in the non-relativistic limit: i.e., when $\lambda \to \infty$.

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001 qfull 00150 3 5 0 tough thinking: Einstein, Runyon

Extra keywords: Bosher

5. "God does not play dice"—Einstein. Discuss.

Chapt. 2 QM Postulates, Schrödinger Equation, and the Wave Function

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Multiple-Choice Problems

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002 qmult 00080 1 1 2 easy memory: wave-particle duality

1. The nebulous (and sometimes disparaged) concept that all microscopic physical entities have both wave and particle properties is called the wave-particle:

   a) singularity. b) duality. c) triality. d) infinality. e) nullility.

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002 qmult 00090 1 4 5 easy deducto-memory: Sch eqn

2. "Let's play *Jeopardy*! For \$100, the answer is: The equation that governs (or equations that govern) the time evolution of quantum mechanical systems in the non-relativistic approximation."

   What is/are ____________, Alex?

   a) $\vec{F}_{\text{net}} = m\vec{a}$ b) Maxwell's equations
   c) Einstein's field equations of general relativity d) Dirac's equation
   e) Schrödinger's equation

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002 qmult 00100 1 1 1 easy memory: Sch eqn compact form

3. The full Schrödinger's equation in compact form is:

   a) $H\Psi = i\hbar\frac{\partial\Psi}{\partial t}$. b) $H\Psi = \hbar\frac{\partial\Psi}{\partial t}$. c) $H\Psi = i\frac{\partial\Psi}{\partial t}$. d) $H\Psi = i\hbar\frac{\partial\Psi}{\partial x}$.
   e) $H^{-1}\Psi = i\hbar\frac{\partial\Psi}{\partial t}$.

---

002 qmult 00110 1 1 3 easy memory: Hamiltonian operator

4. The energy operator in quantum mechanics,

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

   (here given for 1 particle in one dimension) is called the:

   a) Lagrangian b) Laplacian c) Hamiltonian d) Georgian e) Torontonian

---

002 qmult 00200 1 4 3 easy deducto-memory: Born postulate
Extra keywords: mathematical physics

5. "Let's play *Jeopardy*! For \$100, the answer is: The postulate that the wave function $\Psi(\vec{r})$ is quantum mechanics is a probability amplitude and $|\Psi(\vec{r})|^2$ is a probability density for localizing a particle at $\vec{r}$ on a 'measurement'."

   What is ____________, Alex?

   a) Schrödinger's idea b) Einstein's notion c) Born's postulate
   d) Dirac's hypothesis e) Death's conclusion

---

002 qmult 00210 1 1 1 easy memory: QM probability density

6. In the probabilistic interpretation of wave function Ψ, the quantity $|\Psi|^2$ is:

a) a probability density. b) a probability amplitude. c) 1. d) 0.
e) a negative probability.

---

002 qmult 00220 1 1 5 easy memory: probability of finding particle in dx

7. The probability of finding a particle in differential region dx is:

a) $\Psi(x,t)\,dx$. b) $\Psi(x,t)^*\,dx$. c) $[\Psi(x,t)^*/\Psi(x,t)]\,dx$. d) $\Psi(x,t)^2\,dx$.
e) $\Psi(x,t)^*\Psi(x,t)\,dx = |\Psi(x,t)|^2\,dx$.

---

002 qmult 00300 1 4 5 easy deducto-memory: observable defined
Extra keywords: See Co-137, Gr-104

8. "Let's play *Jeopardy*! For $100, the answer is: It is an Hermitian operator that governs (or represents in some people's jargon) a dynamical variable in quantum mechanics."

What is an ____________, Alex?

a) intangible b) intaglio c) obtainable d) oblivion e) observable

---

002 qmult 00310 1 1 3 easy memory: expectation value defined

9. In quantum mechanics, a dynamical variable is governed by a Hermitian operator called an observable that has an expectation value that is:

a) the most likely value of the quantity given by the probability density: i.e., the mode of the probability density.
b) the median value of the quantity given by the probability density.
c) the mean value of the quantity given by the probability density.
d) any value you happen to measure.
e) the time average of the quantity.

---

002 qmult 00320 1 1 3 easy memory: expectation value notation

10. The expectation value of operator Q for some wave function is often written:

a) Q. b) $\rangle Q\langle$. c) $\langle Q\rangle$. d) $\langle f(Q)\rangle$. e) $f(Q)$.

---

002 qmult 00400 1 1 1 easy memory: physical requirments
Extra keywords: Gr-11

11. These quantum mechanical entities must be (with some exceptions):

i) Single-valued (and their derivatives too).
ii) finite (and their derivatives too).
iii) continuous (and their derivatives too).
iv) normalizable or square-integrable.

They are:
a) wave functions. b) observables. c) expectation values. d) wavelengths.
e) wavenumbers.

---

002 qmult 00410 1 1 4 easy memory: normalization requirement

12. A physical requirement on wave functions is that they should be:

a) reliable. b) friable. c) certifiable. d) normalizable. e) retriable.

---

002 qmult 00500 1 1 2 easy memory: the momentum operator defined

13. The momentum operator in one-dimension is:

a) $\hbar\dfrac{\partial}{\partial x}$. b) $\dfrac{\hbar}{i}\dfrac{\partial}{\partial x}$. c) $\dfrac{i}{\hbar}\dfrac{\partial}{\partial x}$. d) $\dfrac{i}{\hbar}\dfrac{\partial}{\partial t}$. e) $\hbar\dfrac{\partial}{\partial t}$.

---

002 qmult 00510 1 1 4 easy memory: constant of the motion

14. If an observable has no explicit time dependence and it commutes with the Hamiltonian, then it is a quantum mechanical:

a) fudge factor. b) dynamical variable. c) universal constant.
d) constant of the motion. e) constant of the stagnation.

---

002 qmult 00520 1 4 5 easy deducto-memory: Ehrenfest's theorem

15. Ehrenfest's theorem partially shows the connection between quantum mechanics and:

a) photonics. b) electronics. c) special relativity. d) general relativity.
e) classical mechanics.

---

002 qmult 00600 1 4 5 easy deducto-memory: uncertainty principle 1

16. "Let's play *Jeopardy*! For $100, the answer is: It describes a fundamental limitation on the accuracy with which we can know position and momentum simultaneously."

What is ____________, Alex?

a) Tarkovsky's doubtful thesis b) Rublev's ambiguous postulate
c) Kelvin's nebulous zeroth law d) Schrödinger's wild hypothesis
e) Heisenberg's uncertainty principle

---

002 qmult 00610 1 4 5 easy deducto-memory: uncertainty principle 2

17. "Let's play *Jeopardy*! For $100, the answer is: $\Delta x \Delta p \geq \hbar/2$ or $\sigma_x \sigma_p \geq \hbar/2$.

What is ____________, Alex?

a) an equality b) a standard deviation
c) the Heisenberg **CERTAINTY** principle d) the Cosmological principle
e) the Heisenberg **UNCERTAINTY** principle

---

002 qmult 00700 1 1 4 easy memory: Schr. eqn. separation of variables

18. The time-independent Schrödinger equation is obtained from the full Schrödinger equation by:

a) colloquialism. b) solution for eigenfunctions.
c) separation of the x and y variables. d) separation of the space and time variables.
e) expansion.

---

002 qmult 00720 1 1 1 easy memory: stationary state

19. A system in a stationary state will:

a) not evolve in time. b) evolve in time. c) both evolve and not evolve in time.
d) occasionally evolve in time. e) violate the Heisenberg uncertainty principle.

---

002 qmult 00800 1 4 2 easy deducto-memory: orthogonality property

20. For a Hermitian operator eigenproblem, one can always find (subject to some qualitifications perhaps—but which are just mathemtical hemming and hawwing) a complete set (or basis) of eigenfunctions that are:

a) independent of the x-coordinate. b) orthonormal. c) collinear.
d) pathological. e) righteous.

---

002 qmult 00810 1 4 2 easy deducto-memory: basis expansion
Extra keywords: mathematical physics

21. "Let's play *Jeopardy*! For $100, the answer is: If it shares the same same range as a basis set of functions and is at least piecewise continuous, then it can be expanded in the basis with a vanishing limit of the mean square error between it and the expansion."

What is a/an ____________, Alex?

a) equation b) function c) triangle d) deduction e) tax deduction

---

002 qmult 00820 1 4 5 easy deducto-memory: general Born postulate
Extra keywords: mathematical physics

22. "Let's play *Jeopardy*! For \$100, the answer is: The postulate that expansion coefficients of a wave function in the eigenstates of an observable are the probability amplitudes for wave function collapse to eigenstates of that observable."

    What is ____________, Alex?

    a) the special Born postulate b) the very special Born postulate
    c) normalizability d) the mass-energy equivalence e) the general Born postulate

---

002 qmult 00830 1 1 4 easy memory: basis expansion physics

23. The expansion of a wave function in an observable's basis (or complete set of eigenstates) is

    a) just a mathematical decomposition. b) useless in quantum mechanics.
    c) irrelevant in quantum mechanics. d) not just a mathematical decomposition since the expansion coefficients are probability amplitudes. e) just.

---

020 qmult 00840 1 4 5 easy deducto-memory: wave function collapse

Extra keywords: mathematical physics

24. "Let's play *Jeopardy*! For \$100, the answer is: It is a process in quantum mechanics that some decline to mention, some believe to be unspeakable, some believe does not exist (though they have got some explaining to do about how one ever measures anything), some believe should not exist, and that some call the fundamental perturbation (but just once per textbook)."

    What is ____________, Alex?

    a) the Holy b) the Unholy c) the Unnameable
    d) the 4th secret of the inner circle e) wave function collapse

---

002 qmult 00900 1 4 1 easy deducto-memory: macro object in stationary state

25. "Let's play *Jeopardy*! For \$100, the answer is: A state that no macroscopic system can be in except arguably for states of Bose-Einstein condensates, superconductors, superfluids and maybe others sort of."

    What is a/an ____________, Alex?

    a) stationary state b) accelerating state c) state of the Union d) state of being
    e) state of mind

---

002 qmult 01000 1 1 5 easy memory: stationary state is radical

26. A stationary state is:

    a) just a special kind of classical state. b) more or less a kind of classical state.
    c) voluntarily a classical state.
    d) was originally not a classical state, but grew into one.
    e) radically unlike a classical state.

---

002 qmult 01100 1 1 4 easy memory: macro system in a stationary state

27. Except arguably for certain special cases (superconductors, superfluids, and Bose-Einstein condensates), no macroscopic system can be in a:

    a) mixed state. b) vastly mixed state. c) classical state. d) stationary state.
    e) state of the union.

---

002 qmult 01200 1 1 2 easy memory: transitions

28. Transitions between atomic or molecular stationary states (sometimes, but actually rarely, called quantum jumps) are:

    a) only collisional.
    b) both collisional and radiative.
    c) only radiative.

d) neither collisional nor radiative.
e) only collisional to higher energy stationary states and only radiative to lower energy stationary states.

---

002 qmult 01300 1 4 3 easy deducto-memory: lasers, stimulated emission

29. "Let's play *Jeopardy*! For \$100, the answer is: It is the basis for lasers and masers."

What is ____________, Alex?

a) spontaneous radiative emission b) desultory radiative emission
c) stimulated radiative emission d) the laser force e) the laser potential

---

002 qmult 01400 1 4 4 easy deducto-memory: operators and Sch. eqn.

30. "Let's play *Jeopardy*! For \$100, the answer is: An equation that must hold in order for the non-relativistic Hamiltonian operator and the operator $i\hbar\partial/\partial t$ to both yield an energy expectation value for a wave function $\Psi(x,t)$."

What is ____________, Alex?

a) the continuity equation b) the Laplace equation c) Newton's 2nd law
d) Schrödinger's equation e) Hamiton's equation

---

002 qmult 02000 2 1 4 moderate memory: does gravity quantize
Extra keywords: reference: Nesvizhevsky et al. 2002, Nature, 413, 297

31. Can the gravitational potential cause quantization of energy states?

a) No. b) It is completely uncertain. c) Theoretically yes, but experimentally no.
d) Experimental evidence to date (post-2001) suggests it can.
e) In principle there is no way of telling.

Full-Answer Problems

002 qfull 00090 1 5 0 easy thinking: what is a wave function?

1. What is a wave function? (Representative general symbol $\Psi(\vec{r},t)$).

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002 qfull 00100 1 3 0 easy math: probability and age distribution
Extra keywords: (Gr-10:1.1)

2. Given the following age distribution, compute its the normalization (i.e., the factor that normalizes the distribution), mean, variance, and standard deviation. Also give the mode (i.e., the age with highest frequency) and median. **HINT:** Doing the calculation with a small computer code would be the efficient way to answer the problem.

Table: Age Distribution

Age (years)	Frequency
14	2
15	1
16	6
22	2
24	2
25	5

002 qfull 00200 2 3 0 moderate math: probability needle 1

Extra keywords: (Gr-10:1.3) probability and continuous variables

3. An indicator needle on a semi-circular scale (e.g., like a needle on car speedometer) bounces around and comes to rest with equal probability at any angle θ in the interval $[0, \pi]$.

   a) Give the probability density $\rho(\theta)$ and sketch a plot of it.

   b) Compute the 1st and 2nd moments of the distribution (i.e., $\langle\theta\rangle$ and $\langle\theta^2\rangle$) and the variance and standard deviation.

   c) Compute $\langle\sin\theta\rangle$, $\langle\cos\theta\rangle$, $\langle\sin^2\theta\rangle$, and $\langle\cos^2\theta\rangle$.

---

002 qfull 00210 3 5 0 tough thinking: 2-variable probability density

Extra keywords: (Gr-11:1.5) dropping a needle on lines needle 2

4. Nun für eine kleine teufelische problem. Say you drop at random with equal likelihood of landing in any orientation and location a needle of length ℓ onto a sheet of paper with parallel lines a distance ℓ apart. What is the probability of the needle crossing (or at least touching) a line? Let's be nice this time and break it down.

   a) Mentally mark one end of needle red. Then note that really we only need to consider one band on the paper between two parallel lines and the case where the red end lies between them as a given. Why is this so?

   b) So now we consider that the red end lands in one band at a point x between $-\ell/2$ and $\ell/2$. Note we put the origin at the center since almost always one ought to exploit symmetry. What is the probability density for the red end to land anywhere in the band? What is the probability density for the needle for the orientation of the needle in θ measured from the x-axis? Why do you only need to consider $\theta \in [0, \pi]$?

   c) Now we don't care about the orientation itself really: we just care about it's projection on the x-axis. Call that projection x'. What is the probability density for x'? What is the range of x' allowed? **HINT:** The probability of landing in $d\theta$ and a corresponding dx' must be equal.

   d) The joint probability density for x and x' is

   $$\rho(x)\rho(x') \ .$$

   You now have to integrate up all the probability for $x' + x \geq \ell/2$ and for $x' + x \leq -\ell/2$ and sum those two probabilities. The sum is the solution probability of course.

---

002 qfull 00220 1 3 0 easy math: Gaussian probability density

Extra keywords: (Gr-11:1.6)

5. Consider the Gaussian probability density

   $$\rho(x) = Ae^{-\lambda(x-a)^2} \ ,$$

   where A, a, and λ are constants.

   a) Determine the normalization constant A.

   b) The nth moment of a probability density is defined by

   $$\langle x^n \rangle = \int_{-\infty}^{\infty} x^n \rho(x)\, dx \ .$$

   Determine the 0th, 1st, and 2nd moments of the Gaussian probability density.

c) For the Gaussian probability density determine the mean, mode, mediam, variance σ^2, and standard deviation (or dispersion) σ.

d) Sketch the Gaussian probability density.

---

002 qfull 00300 2 3 0 moderate math: analyzing a triangular hat wave function

Extra keywords: (Gr-13:1.7)

6. At some time a triangular hat wave function is given by

$$\Psi(x,t) = \begin{cases} A\dfrac{x}{a} \ , & x \in [0,a]; \\[2ex] A\left(\dfrac{b-x}{b-a}\right) \ , & x \in [a,b]; \\[2ex] 0 & \text{otherwise,} \end{cases}$$

where A, a, and b are constants.

a) Sketch Ψ and locate most probable location for a particle (i.e., the mode of the $|\Psi|^2$ probability distribution).

b) Determine the normalization constant A in terms of a and b. Recall the difference between wave function and probability distribution here and in the later parts of this question.

c) What are the probabilities of being found left and right of a, respectively?

d) What is $\langle x\rangle$?

---

002 qfull 00310 2 5 0 moderate thinking: probability conservation

Extra keywords: (Gr-13:1.9) probability current

7. The expression for the probability that a particle is in the region $[-\infty, x]$ (i.e., the cumulative probability distribution function) is

$$P(x,t) = \int_{-\infty}^{x} |\Psi(x',t)|^2 \, dx' \ .$$

a) Find an explicit, non-integral formula for $\partial P(x,t)/\partial t$ given that the wave function is normalizable at time t. Simplify the formula as much as reasonably possible. **HINT:** Make use of the physics: i.e., the Schrödinger equation itself. This is a common trick in quantum mechanics and, *mutatis mutandis*, throughout physics. It probably helps to let the dummy variable in the integral be x and the endpoint a while doing the math.

b) Recall momentum observable is

$$p_{\rm op} = \frac{\hbar}{i}\frac{\partial}{\partial x} \ .$$

Substitute $p_{\rm op}$ into the formula derived in part (a) and simplify as much as possible. In the simplification, make use of the real-part function Re which has the property that

$$\mathrm{Re}(z)$$

is the real part of complex variable z. For example, if $z = x + iy$, then

$$\mathrm{Re}(z) = \mathrm{Re}(x+iy) = x \ .$$

HINT: Note that

$$-p_{\rm op}\Psi^* = (p_{\rm op}\Psi)^* \ .$$

c) If the wave function is normalizable at time t, show that $P(\infty, t)$ is a constant with respect to time: i.e., total probability is conserved.

d) The probability current is defined

$$J(x,t) = -\frac{\partial P(x,t)}{\partial t} \; .$$

Argue that this is a sensible definition. Then using the part (b) answer write an explicit formula for $J(x,t)$ in terms of the wave function. Discuss how this formula corresponds to a classical current density: e.g.,

$$\vec{v}\rho$$

where $\vec{v}$ is velocity and ρ is a density of something.

e) Given

$$\Psi(x,t) = \psi(x)e^{-i\omega t} \; ,$$

what can one say about the probability density $|\Psi|^2$, the cumulative probability function $P(x,t)$, and the probability current $J(x,t)$?

---

002 qfull 00320 3 5 0 tough thinking: general time evolution equation

8. It follows from the general Born postulate that the expectation value of an observable Q is given by

$$\langle Q \rangle = \int_{-\infty}^{\infty} \Psi^* Q \Psi \, dx \; .$$

It's weird to call an operator an observable, but that is the convention (Co-137).

a) Write down the explicit expression for

$$\frac{d\langle Q \rangle}{dt} \; .$$

Recall Q in general can depend on time too.

b) Now use the Schrödinger equation

$$H\Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

to eliminate partial time derivatives where possible in the expression for $d\langle Q \rangle / dt$. Remember how complex values behave when complex conjugated. You should use the angle bracket form for expectation values to simplify the expression where possible.

c) The commutator of two operators A and B is defined by

$$[A,B] = AB - BA \; ,$$

where it is always understood that the commutator and operators are acting on an implicit general function to the right. If you have trouble initially remembering the understood condition, you can write

$$[A,B]f = (AB - BA)f \; ,$$

where f is an explicit general function. Operators don't in general commute: i.e., $[A,B] = AB - BA \neq 0$ in general. Prove

$$\left[\sum_i A_i, \sum_j B_j \right] = \sum_{i,j} [A_i, B_j] \; .$$

d) Now show that $d\langle Q\rangle/dt$ can be written in terms of $\langle i[H,Q]\rangle$. The resulting important expression oddly enough doesn't seem to have a common name. I just call it the general time evolution formula. **HINTS:** First, V and Ψ^* do commute. Second, the other part of the Hamiltonian operator

$$T = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

can be put in the right place using integration by parts and the normalization condition on the wave function. Note T turns out to be the kinetic energy operator.

e) If $d\langle Q\rangle/dt = 0$, then Q is a quantum mechanical constant of the motion. It's weird to call an observable (which is a operator) a constant of the motion, but that is the convention (Co-247). Show that the operator $Q = 1$ (i.e., the unit operator) is a constant of the motion. What is $\langle 1\rangle$?

f) Find the expression for $d\langle x\rangle/dt$ in terms of what we are led to postulate as the momentum operator

$$p = \frac{\hbar}{i}\frac{\partial}{\partial x} .$$

The position operator x should be eliminated from the expression. **HINTS:** Note V and x commute, but T and x do not. Leibniz's formula (Ar-558) might be of use in evaluating the commutator $[T,x]$. The formula is

$$\frac{d^n(fg)}{dx^n} = \sum_{k=0}^{n}\binom{n}{k}\frac{d^k f}{dx^k}\frac{d^{n-k}g}{dx^{n-k}} .$$

---

002 qfull 00330 3 5 0 tough thinking: Ehrenfest's theorem

Extra keywords: (Gr-17:1.12) Ehrenfest formulae

9. In one dimension, Ehrenfest's theorem in quantum mechanics is usually taken to consist of two formulae:

$$\frac{d\langle x\rangle}{dt} = \frac{1}{m}\langle p\rangle$$

and

$$\frac{d\langle p\rangle}{dt} = -\left\langle \frac{\partial V}{\partial x}\right\rangle ,$$

where the angle brackets indicate expectation values as usual.

NOTE: There are parts a,b,c,d. The parts can all be done independently. So don't stop if you can't do a part.

a) From the general time evolution formula prove the 1st Ehrenfest formula. **HINTS:** Recall the general time evolution formula in non-relativistic quantum mechanics is

$$\frac{d\langle Q\rangle}{dt} = \left\langle \frac{\partial Q}{\partial t}\right\rangle + \frac{1}{\hbar}\langle i[H,Q]\rangle ,$$

where Q is any observable and H is the Hamiltonian:

$$H = T + V(x) .$$

Also recall that quantum mechanical momentum operator and kinetic energy operator are given by

$$p = \frac{\hbar}{i}\frac{\partial}{\partial x} \qquad \text{and} \qquad T = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} ,$$

respectively. Leibniz's formula (Ar3-667) might be of use in evaluating some of the commutators:

$$\frac{d^n(fg)}{dx^n} = \sum_{k=0}^{n} \binom{n}{k} \frac{d^k f}{dx^k} \frac{d^{n-k} g}{dx^{n-k}} .$$

b) From the general time evolution formula prove the 2nd Ehrenfest formula.

c) In the macroscopic limit, the expectation values become the classical dynamical variables by the correspondence principle (which is an auxiliary principle of quantum mechanics enunciated by Bohr in 1920 (Wikipedia: Correspondance principle)): i.e., $\langle x \rangle$ becomes x, etc. (Note we are allowing a common ambiguity in notation: x and p are both coordinates and, in the classical formalism, the dynamical variables describing the particle. Everybody does this: who are we to disagree.) Find the macroscopic limits of the Ehrenfest formulae and identify the macroscopic limits in the terminology of classical physics.

d) If you **ARE** writing a **TEST**, omit this part.

If one combines the two Ehrenfest formulae, one gets

$$m \frac{d^2 \langle x \rangle}{dt^2} = -\left\langle \frac{\partial V}{\partial x} \right\rangle$$

which looks very like Newton's 2nd law in its $F = ma$ form for a force given by a potential. Using the correspondence priniciple, it does become the 2nd law in the macroscopic limit. However, an interesting question arises—well maybe not all that interesting—does the $\langle x \rangle$ (which we could call the center of the wave packet) actually obey the 2nd law-like expression

$$m \frac{d^2 \langle x \rangle}{dt^2} = -\frac{\partial V(\langle x \rangle)}{\partial \langle x \rangle} \ ?$$

To disprove a general statement, all you need to do is find one counterexample. Consider a potential of the form $V(x) = Ax^\lambda$, and show that in general the $\langle x \rangle$ doesn't obey 2nd law-like expression given above. Then show that it does in three special cases of λ.

---

002 qfull 00400 2 3 0 moderate math: orthonormality leads to mean energy

Extra keywords: (Gr-30:2.10)

10. You are given a complete set of orthonormal stationary states (i.e., energy eigenfunctions) $\{\psi_n\}$ and a general wave equation $\Psi(x,t)$ that is for the same system as $\{\psi_n\}$: i.e., $\Psi(x,t)$ is detemined by the same Hamiltonian as $\{\psi_n\}$. The set of eigen-energies of $\{\psi_n\}$ are $\{E_n\}$. The system is bounded in space by $x = -\infty$ and $x = \infty$.

   a) Give the formal expansion expression of $\Psi(x,0)$ (i.e., $\Psi(x,t)$ at time zero) in terms of $\{\psi_n\}$. Also give the formal expression for the coefficients of expansion c_n.

   b) Now give the formal expansion for $\Psi(x,t)$ remembering that $\omega_n = E_n/\hbar$. Justify that this is the solution of the Schrödinger equation for the initial conditions $\Psi(x,0)$.

   c) Find the general expression, simplified as far as possible, for expectation value $\langle H^\ell \rangle$ in terms of the expansion coefficients, where ℓ is any positive (or zero) integer. Are these values time dependent?

   d) Give the special cases for $\ell = 0$, 1, and 2, and the expression for the standard deviation for energy σ_E. **HINTS:** This should be a very short answer: 3 or 4 lines.

---

002 qfull 00500 3 5 0 tough thinking: real eigen-energies

Extra keywords: (Gr-24:2.1) and all real complete sets

11. There are a few simple theorems one can prove about stationary states and their eigen-energies.

a) Prove that eigen-energies must be real. **HINT:** Prove $\langle H\rangle$ is real for any state Ψ using integration by parts. Note one has to use the full time dependent wave function for a general state since the time dependence doesn't cancel out of the expectation value integral.

b) The complete set of time-independent stationary states you get from a direct solution of the Schrödinger equation may not be all pure real pure. But one can always construct from this complete set another complete set that is all pure real and it is supposedly convenient to do so sometimes—or at least it can be done as a mathematician would say. Show how it can be done. **HINTS:** First note that complete sets are almost always assumed to be minimum complete sets: i.e., each member of the set is independent of all the other members, and thus cannot be constructed from any linear combination of the others. In our discussions we always assume minimum complete sets.

Consider a non-trivially complex solution ψ_{ij} of the eigenproblem

$$H\psi_{ij} = E_i\psi_{ij} \ ,$$

where the first subscript denotes energy level and the second the particular solution of that energy level. ("Non-trivially" just means that ψ_{ij} isn't just a real function times a complex constant. What do you do with a trivially complex ψ_{ij} by the way?) Take the complex conjugate of the eigenproblem to find an independent 2nd solution $\psi_{\rm 2nd}$ to it with the same energy. The 2nd solution may or may not be part of your original subset with energy E_i. If it is, then that is good. But if it isn't one of the original subset with energy E_i, you should replace one of those with $\psi_{\rm 2nd}$. Since the original set was complete

$$\psi_{\rm 2nd} = \sum_\ell c_\ell \psi_{i\ell} \ ,$$

where the summation only needs to run over the eigenfunctions with the same energy E_i. This equation can be rearranged for any ψ_{im} (except for ψ_{ij} itself):

$$\psi_{im} = \sum_\ell c_{\ell\neq m}\psi_{i\ell} + c\psi_{\rm 2nd} \ ,$$

where the coefficients c_ℓ all had to be changed and c is the coefficient needed for $\psi_{\rm 2nd}$. Since ψ_{im} can be constructed using $\psi_{\rm 2nd}$, it can be replaced by $\psi_{\rm 2nd}$. If the number of states with energy E_i is infinite, the replacement process becomes hairy, but let's not worry about that.

Now construct two pure real solutions from ψ_{ij} and $\psi_{\rm 2nd}$ from which ψ_{ij} and $\psi_{\rm 2nd}$ can be re-constructed. These two new states then replace ψ_{ij} and $\psi_{\rm 2nd}$ in the subset with energy E_i. One can go on like that replacing two for two as long as you need to. Remember the original set will in general be infinite, and one couldn't have had them all explicitly anyway.

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002 qfull 00600 3 5 0 tough thinking: parity operator

12. The parity operator P (not to be confused with the momentum operator p) has the well defined, but seemingly arbitrary, property that

$$Pf(x) = f(-x)$$

for a 1-dimensional case which is all that we will consider in this problem.

a) Prove the parity operator is Hermitian. **HINTS:** Recall that the definition of the Hermitian conjugate of operator Q is

$$\langle\phi|Q|\psi\rangle = \langle\psi|Q^\dagger|\phi\rangle^* \ ,$$

where $|\phi\rangle$ and $|\psi\rangle$ are arbitrary kets. Note Q is Hermitian if $Q^\dagger = Q$. Since the parity operator (as defined here) only has meaning in the position representation that is where the proof must be done: thus one must prove

$$\int_{-\infty}^{\infty} \phi(x)^* P\psi(x)\,dx = \left[\int_{-\infty}^{\infty} \psi(x)^* P\phi(x)\,dx\right]^* .$$

A transformation of the integration variable might help: remember x in the integrals is just a dummy variable that can be represented by any symbol.

b) The eigenproblem for the parity operator is

$$Pf(x) = p_{\text{val}} f(x) ,$$

where p_{val} are the eigenvalues. Solve for the complete set of eigenvalues and identify those classes of functions which are eigenfunctions of P. **HINTS:** Note it's $f(x)$ on the right hand side not $f(-x)$ since this is an eigenproblem, but $Pf(x) = f(-x)$ too. Recall that the eigenvalues of a Hermitian operator are pure real. Nothing forbids using the parity operator twice. The parity operator commutes with constants of course:

$$P[cf(x)] = cf(-x) = cPf(x) .$$

c) The set of all eigenfunctions of P is complete. Thus P qualifies as an "observable" in QM jargon whether it can be observed or not: i.e., it is a Hermitian operator with a complete set of eigenstates. Show that the set of eigenstates is complete: i.e., that any function $f(x)$ can be written in an expansion of P eigenfunctions. **HINTS:** From any $f(x)$ one can construct another function $f(-x)$ and from $f(x)$ and $f(-x)$ one can construct two eigenfunctions of P, and from those two eigenfunctions of P one can reconstruct ...

d) If $f'(x)$ is the derivative of $f(x)$, then $Pf'(x) = f'(-x)$: i.e., the derivative of $f(x)$ evaluated at $-x$. But what is

$$\frac{\partial}{\partial x}[Pf(x)] \ ?$$

Do P and $\partial/\partial x$ commute? Do P and $\partial^2/\partial x^2$ commute? **HINT:** You've heard of the chain rule.

e) If the potential is even (i.e., $V(x) = V(-x)$) do P and the Hamiltonian H commute? **HINTS:** Recall $PV(x)f(x)$ must be interpreted in QM (unless otherwise clarified) as P acting on the function $V(x)f(x)$ not on $V(x)$ alone.

f) Given that P and H commute and $\psi(x)$ is a solution of the time-independent Schrödinger equation, show that $\psi(-x)$ a solution too with the same eigen-energy as $\psi(x)$: i.e., $\psi(x)$ and $\psi(-x)$ are degenerate eigenstates.

g) Given that P and H commute, show how one can construct from a given complete set of energy eigenstates a complete set of energy eigenstates that are also eigenstates of the parity operator. Assume that the original complete set contains both $\psi(x)$ and $\psi(-x)$: this is not a requirement for finding a common complete set, but it is a simplification here. **HINT:** Recall the part (c) answer.

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002 qfull 01000 2 5 0 moderate thinking: energy and normalization

Extra keywords: (Gr-24:2.2) zero-point energy

13. Classically $E \geq V_{\text{min}}$ for a particle in a conservative system.

a) Show that this classical result must be so. **HINT:** This shouldn't be a from-first-principles proof: it should be about one line.

b) The quantum mechanical analog is almost the same: $\bar{E} = \langle H \rangle > V_{\rm min}$ for any normalizable state of the system considered. Note the equality $\bar{E} = \langle H \rangle = V_{\rm min}$ never holds quantum mechanically. (There is an over-idealized exception, which we consider in part (e).) Prove the inequality. **HINTS:** The key point is to show that $\langle T \rangle > 0$ for all physically allowed states. Use integration by parts.

c) Now show that result $\bar{E} > V_{\rm min}$ implies $E > V_{\rm min}$, where E is any eigen-energy of the system considered. Note the equality $E = V_{\rm min}$ never holds quantum mechanically (except for the over-idealized system considered in part (e)). In a sense, there is no rest state for quantum mechanical particle. This lowest energy is called the zero-point energy.

d) The $E > V_{\rm min}$ result for an eigen-energy in turn implies a 3rd result: any ideal measurement always yields an energy greater than $V_{\rm min}$ Prove this by reference to a quantum mechanical postulate.

e) This part is **NOT** to be done on **EXAMS**: it's just too much (for the grader). There is actually an exception to $E > V_{\rm min}$ result for an eigen-energy where $E = V_{\rm min}$ occurs. The exception is for quantum mechanical systems with periodic boundary conditions and a constant potential. In ordinary 3-dimensional Euclidean space, the periodic boundary conditions can only occur for rings (1-dimensional systems) and sphere surfaces (2-dimensional systems) I believe. Since any real system must have a finite size in all 3 spatial dimensions, one cannot have real systems with only periodic boundary conditions. Thus, the exception to the $E > V_{\rm min}$ result is for unrealistic over-idealized systems. Let us consider the idealized ring system as an example case. The Hamiltonian for a 1-dimensional ring with a constant potential is

$$H = -\frac{\hbar^2}{2mr^2}\frac{\partial^2}{\partial\phi^2} + V ,$$

where r is the ring radius, ϕ is the azimuthal angle, and V is the constant potential. Find the eigen-functions and eigen-energies for the Schrödinger equation for the ring system with periodic boundary conditions imposed. Why must one impose periodic boundary conditions on the solutions? What solution has eigen-energy $E = V_{\rm min}$?

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002 qfull 00110 2 5 0 moderate thinking: beyond the classical turning points

14. The constant energy of a classical particle in a conservative system is given by

$$E = T + V .$$

Since classically $T \geq 0$ always, a bound particle is confined by surface defined by $T = 0$ or $E = V(\vec{r})$. The points constituting this surface are called the turning points: a name which makes most sense in one dimension. Except for static cases where the turning point is trivially the rest point (and maybe some other weird cases), the particle comes to rest only for an instant at a turning point since the forces are unbalanced there. So it's a place where a particle "ponders for an instant before deciding where to go next". The region with $V > E$ is classically forbidden. Now for most quantum mechanical potential wells, the wave function extends beyond the classical turning point surface into the classical forbidden zone and, in fact, usually goes to zero only at infinity. If the potential becomes infinite somewhere (which is an idealization of course), the wave function goes to zero: this happens for the infinite square well for instance.

Let's write the 1-dimensional time-independent Schrödinger equation in the form

$$\frac{\partial^2\psi}{\partial x^2} = \frac{2m}{\hbar^2}(V - E)\psi .$$

a) Now solve for ψ for the region with $V > E$ with simplifying the assumption that V is constant in this region.

b) Can the solutions be normalized?

c) Can the solutions constitute an entire wave function? Can they be part of a wave function? In which regions?

d) Although we assumed constant V, what crudely is the behavior of the wave function likely to be like the regions with $V > E$.

e) For typical potentials considered at our level, qualitatively what is the likelihood of finding the particle in the classically forbidden region? Why?

---

002 qfull 01100 3 5 0 tough thinking: 1-d non-degeneracy

15. If there are no internal degrees of freedom (e.g., spin) and they are **NORMALIZABLE**, then one-particle, 1-dimensional energy eigenstates are non-degenerate. We (that is to say you) will prove this.

Actually, we know already that any 2nd order ordinary linear differential equation has only two linearly independent solutions (Ar-402) which means, in fact, that from the start we know there is a degeneracy of 2 at most. Degeneracy count is the number of independent solutions. If there is more than one independent solution, then infinitely many linear combinations of solutions have the same energy. But in an expansion of wave function, only a set linear independent solutions is needed and thus the number of such solutions is the physically relevant degeneracy. Of course, our proof means that one of the linearly independent solutions is not normalizable.

a) Assume you have two degenerate 1-dimensional energy eigenstates for Hamiltonian H: ψ_1 and ψ_2. Prove that $\psi_1\psi_2' - \psi_2\psi_1'$ equals a constant where the primes indicate derivative with respect to x the spatial variable. **HINT:** Write down the eigenproblem for both ψ_1 and ψ_2 and do some multiplying and subtraction and integration.

b) Prove that the constant in part (a) result must be zero. **HINT:** To be physically allowable eigenstates, the eigenstates must be normalizable.

c) Integrate the result of the part (b) answer and show that the two assumed solutions are not physically distinct. Show for all x that

$$\psi_2(x) = C\psi_1(x) ,$$

where C is a constant. This completes the proof of non-degeneracy since eigenstates that differ by a multiplicative constant are not physically (i.e., expansion) distinct. **HINT:** You have to show that there is no other way than having $\psi_2(x) = C\psi_1(x)$ to satisfy the condition found in the part (b) answer. Remember the eigenproblem is a linear, homogeneous differential equation.

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002 qfull 01200 2 3 0 mod math: 3-d exponential wave function, probability

Extra keywords: (Co1-342:6), 3-d wave function, probability, momentum representation

16. Consider the 3-dimensional wave function

$$\Psi(\vec{r}) = A \exp\left[-\sum_i |x_i|/(2a_i)\right] ,$$

where the sum runs over the three Cartesian coordinates and the a_i's are real positive length parameters.

a) Calculate the normalization factor A. **HINT:** Recall that the integrand is $|\Psi(\vec{r})|^2 = \Psi(\vec{r})^*\Psi(\vec{r})$. I'm always forgetting this myself when the function is pure real and there is no imaginary part to remind me of it.

b) Calculate the probability that a measurement of x_i will yield a result between 0 and a_i, where i could be any of the three coordinates. **HINT:** There are no restrictions on values of the other coordinates: they could be anything at all. Thus one just integrates over all of those other coordinate positions remembering normalization of course.

c) Calculate the probability that simultaneous measurements of x_j and x_k will yield results in the ranges $-a_j$ to a_j and $-a_k$ to a_k, respectively. The j and k could be any pair of the two coordinates. **HINT:** Remember the hint for part (b).

d) Calculate the probability that a measurment of momentum will yield a result in the element $dp_i\, dp_j\, dp_k$ centered at the point $p_i = p_j = 0$, $p_k = \hbar/a_k$. **HINT:** You will need to find the momentum representation of the state.

Chapt. 3 Infinite Square Wells and Other Wells

Multiple-Choice Problems

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003 qmult 00050 1 1 1 easy memory: infinite square well

1. In quantum mechanics, the infinite square well can be regarded as the prototype of:

   a) all bound systems. b) all unbound systems.
   c) both bound and unbound systems. d) neither bound nor unbound systems.
   e) Prometheus unbound.

---

003 qmult 00100 2 4 2 moderate deducto-memory: infinite square well BCs

2. In the infinite square well problem, the wave function and its first spatial derivative are:

   a) both continuous at the boundaries.
   b) continuous and discontinuous at the boundaries, respectively.
   c) both discontinuous at the boundaries.
   d) discontinuous and continuous at the boundaries, respectively.
   e) both infinite at the boundaries.

---

003 qmult 00300 1 1 3 easy memory: boundary conditions

3. Meeting the boundary conditions of bound quantum mechanical systems imposes:

   a) Heisenberg's uncertainty principle. b) Schrödinger's equation. c) quantization.
   d) a vector potential. e) a time-dependent potential.

---

003 qmult 00400 1 1 5 easy memory: continuum of unbound states

4. At energies higher than the bound stationary states there:

   a) are between one and several tens of unbound states.
   b) are only two unbound states. c) is a single unbound state. d) are no states.
   e) is a continuum of unbound states.

---

003 qmult 00500 1 4 2 easy deducto-memory: tunneling

5. "Let's play *Jeopardy*! For $100, the answer is: This effect occurs because wave functions can extend (in an exponentially decreasing way albeit) into the classically forbidden region: i.e., the region where a classical particle would have negative kinetic energy."

   What is ____________, Alex?

   a) stimulated radiative emission b) quantum mechanical tunneling c) quantization
   d) symmetrization e) normalization

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003 qmult 00600 2 1 2 moderate memory: benzene ring model

6. A simple model of the outer electronic structure of a benzene molecule is a 1-dimensional infinite square well with:

   a) vanishing boundary conditions. b) periodic boundary conditions.
   c) aperiodic boundary conditions. d) no boundary conditions.
   e) incorrect boundary conditions.

Full-Answer Problems

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003 qfull 00100 2 3 0 moderate math: infinite square well in 1-d

1. You are given the time-independent Schrödinger equation

$$H\psi(x) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\psi(x)$$

and the infinite square well potential

$$V(x) = \begin{cases} 0\,, & x \in [0,a]; \\ \infty & \text{otherwise.} \end{cases}$$

NOTE: There are parts a,b,c,d,e,f,g.

a) What must the wave function be outside of the well (i.e., outside of the region $[0,a]$) in order to satisfy the Schrödinger equation? Why?

b) What boundary conditions must the wave function satisfy? Why must it satisfy these boundary conditions?

c) Reduce Schrödinger's equation inside the well to an equation of the same form as the **CLASSICAL** simple harmonic oscillator differential equation with all the constants combined into a factor of $-k^2$, where k is newly defined constant. What is k's definition?

d) Solve for the general solution for a **SINGLE** k value, but don't impose boundary conditions or normalization yet. A solution by inspection is adequate. Why can't we allow solutions with $E \leq 0$? Think carefully: it's not because k is imaginary when $E < 0$.

e) Use the boundary conditions to eliminate most of the solutions with $E > 0$ and to impose quantization on the allowed set of distinct solutions (i.e., on the allowed k values). Give the general wave function with the boundary conditions imposed and give the quantization rule for k in terms of a dimensionless quantum number n. Note that the multiplication of a wave function by an arbitrary global phase factor $e^{i\phi}$ (where ϕ is arbitrary) does not create a physically distinct wave function (i.e., does not create a new wave function as recognized by nature.) (Note the orthogonality relation used in expanding general functions in eigenfunctions also does not distinguish eigenfunctions that differ by global phase factors either: i.e., it gives the expansion coefficients only for distinct eigenfunctions. So the idea of distinct eigenfunctions arises in pure mathematics as well as in physics.)

f) Normalize the solutions.

g) Determine the general formula for the eigenenergies in terms of the quantum number n.

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003 qfull 00100 2 3 0 moderate math: Continuity properties of wave function.

2. Herein we consider the continuity properties of the wave function and its 1st derivative at some length. We will first only consider stationary states. We'll briefly consider non-stationary states afterward. The only problem is to decide if there is any sense in the whole farrago.

We recall that the wave function must be normalizable: i.e.,

$$\int_{-\infty}^{\infty} |\psi|^2\,dx$$

must be non-infinite. This implies that the wave function (both real and imaginary parts) cannot be infinite over any finite range (i.e., over any region bigger than a point). If it were infinite over any finite range, then it would not be normalizable.

What about the wave function going to infinity at a point. Normalization doesn't rule that out completely. There are functions with infinities that integrate to a finite value: e.g., the derivative of $\pm\sqrt{\pm x}$ (with upper case for $x > 0$ and lower case for $x < 0$) has such infinity at $x = 0$). But let's rule those pathological cases that are unlikely to turn up physically or even in useful limiting cases. There is an exception, of course. We allow Dirac delta wave functions, but only as position eigenstates that a particle cannot actually be in.

Now what of infinite potentials and infinite eigenenergies? They probably do not exist in any real sense. But infinite potentials are useful limiting cases of very large real potentials, and so we will consider them below. There seems no reason to consider states with infinite eigenenergies even as limiting cases.

Now for the continuity conditions for non-infinite potentials. First note that the time independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\psi'' + V\psi = E\psi$$

can be rewritten as

$$\psi'' = \frac{2m}{\hbar^2}(V - E)\psi \ .$$

We allow V to have discontinuities, but no infinities. Maybe some real potentials do have discontinuities in some sense, but in any case potentials with discontinuities are useful limiting cases of potentials with very steep regions. At first we cannot rule out discontinuities in ψ. From the rewritten Schrödinger equation, we see that ψ'' can have no infinities though it can have discontinuities at least from those we allow in the potential. This means that ψ' has no discontinuities since they would generate infinities in ψ''. So ψ' is continuous. But ψ' is allowed to have kinks.

Here we define kink to be a place where the function is continuous, but the derivative is not. So kinks in the ψ' mean discontinuities in ψ''. There must be genuine math term for "kink", but I can't locate it nohow. It's not "cusp" anyway.

Now any kinks in ψ would cause discontinuities in ψ'. So ψ can have no kinks.

I think there is no non-pathological way that ψ can have a kinkless discontinuity without leading to infinity in ψ''. So ψ has to be continuous. And I think there is no non-pathological way that ψ' can have continuous infinity without leading to an infinity in ψ''. So I think ψ' can have no infinities.

The upshot is that without pathological cases, ψ and ψ' should be continuous and non-infinite everywhere where the potential is non-infinite. And ψ'' can have discontinuities, but no infinities.

If one encounters pathological cases, one probably must deal with them on a case by case basis.

As aforementioned, as idealized limit we do invoke infinite potentials both over finite regions (as in the infinite square well case) and at points. What the continuity conditions in these cases?

First what happens to ψ if V goes to infinity over a finite range? Consider the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\psi'' + V\psi = E\psi \ .$$

Say V becomes infinite over the finite range. The only way for Schrödinger equation to be satisfied with ψ and ψ'' not allowed to be infinite over the finite range and E staying non-infinite is to make ψ (and therefore ψ'') zero over the range. Note that it would require a very pathological ψ to non-infinite over the range, but have ψ'' infinite over the range. In fact, we don't need to consider such pathological ψ's for any reason I think.

So we take it that if V is infinite over a finite range, ψ is zero in that range.

Inside a finite range of infinite V, ψ and ψ' must be zero and therefore are continouts. Outside of the range V is finite and we have our earlier result that ψ and ψ' are continuous. What about at the position where V goes from being finite to infinite? Let's call the position the potential wall. To analyze the continuity conditions are the potential wall let's say the wall is at $x = 0$ (without loss of generality) and start by saying that the potential for $x < 0$ is a finite V_- and the potential for $x > 0$ is a finite V. There is a discontinuity in potential at the potential wall and we will let V_-

go to infinity and become our infinite potential. On both sides of the wall, there are small regions where the potential can be approximated as constant.

Let's find the general solution for time-independent Schrödinger equation for a small enough region that V can be approximated as constant in it. We can rewrite the time-independent Schrödinger equation to the form

$$\psi'' = \kappa^2\psi \ ,$$

where we define

$$\kappa = \sqrt{\frac{2m}{\hbar^2}(V-E)} \ .$$

Note that if $E > V$, then

$$\kappa = ik \ ,$$

where

$$k = \sqrt{\frac{2m}{\hbar^2}(E-V)} \ .$$

Over the sufficiently small region where V can be approximated as a constant, the general solution of Schrödinger equation is

$$\psi = Ae^{\kappa x} + Be^{-\kappa x} \ ,$$

where A and B are set by the full solution for the system (including the boundary conditions) and the normalization condition. If $E = V$ exactly (which must be a so rare as to be negligible case usually),

$$\psi = A + Bx \ .$$

Now as long as V_- is finite, the wave function is non-zero for $x < 0$. From the above solution, *mutatis mutandis*, the solution for the small region just below $x = 0$ is

$$\psi_- = Ce^{\kappa_- x} + De^{-\kappa_- x} \ ,$$

where

$$\kappa_- = \sqrt{\frac{2m}{\hbar^2}(V_- - E)} \ .$$

For the small region just above $x = 0$, we have

$$\psi_+ = Ae^{\kappa x} + Be^{-\kappa x} \ .$$

We are assuming $E \neq V_-$ and $E \neq V$. The former is always OK since we will let V_- go to infinity. The latter is certainly almost always OK, but we will consider the case of $E = V$ exactly below.

Now as long as V_- is finite our original continuity conditions apply and we demand the potential wall conditions

$$C + D = A + B \qquad \text{and} \qquad \kappa_-(C - D) = \kappa(A + B) \ .$$

Note these potential wall conditions just give us two relations between the coefficients A, B, C, and D. We would have to incorporate information from the whole system (including boundary conditions) and impose normalization to determine the coefficients.

Now we let V_- go to infinity. By our earlier considerations, $\psi(x < 0)$ must go to zero. This implies that C goes to zero. Our potential wall conditions are now

$$D = A + B \qquad \text{and} \qquad \lim_{V_- \to \infty} \kappa_-(-D) = \kappa(A + B) \ .$$

Now A, B and κ must be non-infinite and κ_- goes to infinity as V_- go to infinity. Therefore D actually has to go to zero as V_- go to infinity, but in such a way that $\kappa_-(-D)$ is finite and equal to $\psi'_+(0)$. So our potential wall conditions become

$$0 = A + B \qquad \text{and} \qquad \psi'_+(0) = \kappa(A - B) \ .$$

So we find that $B = -A$ and thus that

$$\psi_+ = A(e^{\kappa x} - e^{-\kappa x}) \ , \qquad \psi_+(0) = 0 \ , \qquad \psi'_+(0) = 2\kappa A \ .$$

So the wave function must be continuous as the boundary, but in general the 1st derivative is not.

Note for $V_- = \infty$, we only have a relationship relating A and B. To determine them we would have to incorporate information from the whole system (including boundary conditions) and impose normalization. The determination would also give us $\psi'_+(0)$, of course. It is certainly possible that $\psi'_+(0)$ could turn out to be zero making the 1st derivative zero at $x = 0$, but nothing demands it. In fact, we know from the infinite square well case that $\psi'_+(0)$ does not turn out to be zero in that case at the points where the potential becomes infinite. Actually, it seems that cases where $\psi'_+(0)$ is zero are probably pretty rare. The system would have to be rather fine-tuned to get $\psi'_+(0) = 0$.

There is a kind of conservation of information we note. For V_- non-infinite, we have two relations for wave function and its derivative at the potential wall, but no exact determination of either value. For V_- infinite, we have only one relationship for derivative at the potential wall, but know exactly what the wave function is at the boudnary: it is zero.

Now what of that pesky case of $E = V$ exactly. Well here

$$\psi_+ = A + Bx \ .$$

The potential wall conditions before sending V_- to infinity are

$$C + D = A \qquad \text{and} \qquad \kappa_-(C - D) = B \ .$$

When we send V_- to infinity, C and D go to zero again, D in such a way that $\kappa_-(-D)$ is finite and equal to $\psi'_+(0)$. So we get that $A = 0$, and thus

$$\psi_+ = Bx \ , \qquad \psi_+(0) = 0 \ , \qquad \psi'_+(0) = B \ .$$

So the wave function is continuous at the wall boundary and is zero there and the 1st derivative is not continuous and its value must be determined from the whole solution. The situation is essentially the same as for $E \neq V$ which is not surprising since the $E = V$ case is the limit for the $E < V$ and $E > V$ cases which are both the same as seen by the joint treatment above.

Now for the case that V is infinite at a point.

Well maybe in the 2020s, I'll get to that case. enough is enough right now.

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003 qfull 00400 2 3 0 moderate math: moments of infinite square well

Extra keywords: (Gr-29:2.4)

3. Calculate $\langle x\rangle$, $\langle x^2\rangle$, $\langle p\rangle$, $\langle p^2\rangle$, σ_x, and σ_p for the 1-dimensional infinite square well with range $[0, a]$. Recall the general solution is

$$\psi = \sqrt{\frac{2}{a}}\sin(kx) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) \ ,$$

where $n = 1, 2, 3, \ldots$. Also check that the Heisenberg uncertainty principle is satisfied.

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003 qfull 00450 2 3 0 moderate math: infinite square well features

4. The one-dimensional infinite square well with a symmetric potential and width a is

$$V = \begin{cases} 0 & \text{for } |x| \leq a/2; \\ \infty & \text{for } |x| > a/2. \end{cases}$$

The eigenstates for infinite square well are given by

$$\psi_n(x) = \sqrt{\frac{2}{a}} \times \begin{cases} \cos(kx) & \text{for } n = 1, 3, 5 \ldots; \\ \sin(kx) & \text{for } n = 2, 4, 6 \ldots, \end{cases}$$

where

$$\frac{ka}{2} = \frac{n\pi}{2} \qquad \text{and} \qquad k = \frac{n\pi}{a} \ .$$

The n is the quantum number for eigenstates. The eigenstates have been normalized and are guaranteed orthogonal by the mathematics of Hermitian operators of the which the Hamiltonian is one. A quantum number is a dimensionless index (usually integer or half-integer) that specifies the eigenstates and eigenvalues somehow. The eigen-energies are given by

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 n^2 \ .$$

a) Verify the normalization of eigenstates.

b) Determine $\langle x \rangle$ for the eigenstates.

c) Determine $\langle p_{\rm op} \rangle$ for the eigenstates. **HINT:** Recall

$$p_{\rm op} = \frac{\hbar}{i}\frac{\partial}{\partial x} \ .$$

d) Determine $\langle p_{\rm op}^2 \rangle$ and the momentum standard deviation $\sigma_{\rm p}$ for the eigenstates.

e) Determine $\langle x^2 \rangle$ and the position standard deviation σ_x in the large n limit. **HINT:** Assume x^2 can be approximated constant over one complete cycle of the probability density $\psi_n^*\psi_n$

f) Now for the boring part. Determine $\langle x^2 \rangle$ and the position standard deviation σ_x exactly now. **HINT:** There probably are several different ways of doing this, but there seem to be no quick tricks to the answer. The indefinite integral

$$\int x^2 \cos(bx)\,dx = \frac{x^2}{b}\sin(bx) + \frac{2}{b^2}x\cos(bx) - \frac{2}{b^3}\sin(bx)$$

might be helpful.

g) Verify that the Heisenberg uncertainty principle

$$\Delta x \Delta p = \sigma_x \sigma_p \geq \frac{\hbar}{2}$$

is satisfied for the infinite square well case.

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003 qfull 00500 3 5 0 tough thinking: mixed states of infinite square well

Extra keywords: (Gr-29:2.6)

5. A particle is in a mixed state in a 1-dimensional infinite square well where the well spans $[0, a]$ and the solutions are in the standard form of Gr-26. At time zero the state is

$$\Psi(x, 0) = A\left[\psi_1(x) + \psi_2(x)\right] \ ,$$

where $\psi_1(x)$ and $\psi_2(x)$ are the time-independent 1st and 2nd stationary states of the infinite square well.

a) Determine the normalization constant A. Remember the stationary states are orthonormal. Also is the normalization a constant with time? Prove this from the general time evolution equation

$$\frac{d\langle Q\rangle}{dt} = \left\langle \frac{\partial Q}{\partial t} \right\rangle + \frac{1}{\hbar}\langle i[H,Q]\rangle \ .$$

b) Now write down $\Psi(x,t)$. Give the argument for why it is the solution. As a simplfication in the solution use

$$\omega_1 = \frac{E_1}{\hbar} = \frac{\hbar}{2m}\left(\frac{\pi}{a}\right)^2 \ ,$$

where E_1 is the ground state energy of the infinite square well.

c) Write out $|\Psi(x,t)|^2$ and simplify it so that it is clear that it is pure real. Make use Euler's formula: $e^{ix} = \cos x + i \sin x$. What's different about our mixed state from a stationary state?

d) Determine $\langle x\rangle$ for the mixed state. Note that the solution is oscillatory. What is the angular frequency $w_{\rm q}$ and amplitude of the oscillation. Why would you be wrong if your amplitude was greater than $a/2$.

e) Determine $\langle p\rangle$ for the mixed state. As Peter Lorre (playing Dr. Einstein—Herman Einstein, Heidelberg 1919) said in *Arsenic and Old Lace* "the quick way, Chonny."

f) Determine $\langle H\rangle$ for the mixed state. How does it compare to E_1 and E_2?

g) Say a classical particle had kinetic energy equal to the energy $\langle H\rangle$ found in the part (f) answer. The particle is bounces back and forth between the walls of the infinite square well. What would its angular frequency be in terms of $\omega_{\rm q}$ and the angular frequency found in the part (d) answer.

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003 qfull 00600 2 5 0 moderate thinking: revival time

Extra keywords: Gr-85 The hints make it possible as new test problem.

6. The revival time is the minimum time period for a wave function to repeat (i.e., to cycle back to its original form), or slightly less restrictively, for the probability density to repeat.

a) Say we had a system with eigen-energies given by the formula

$$E_n = E_1 f(n) + E_0 \ ,$$

where E_0 is a zero-point energy, n is a quantum number that runs $1,2,3,\ldots$ or $0,1,2,3,\ldots$, $f(n)$ is a strictly increasing function that always has an integer value, and $f(1) = 1$. What is the revival time (in the probability density sense) for general wave function $\Psi(x,t)$ for this system? **HINT:** The zero-point energy gives a time-dependent global phase factor for any expansion in the stationary states, and thus cancels out of the probability density. Assume orthonormal energy-eigen states and recall

$$\Psi(x,t) = \sum_n c_n e^{-i\omega_n t}\psi_n(x) \ ,$$

where $\omega_n = E_n/\hbar$ are the angular frequencies and $\psi_n(x)$ are the energy-eigenstates. The period for ω_n is $2\pi/\omega_n$.

b) The eigen-energies for the infinite square well and the simple harmonic oscillator are, respectively,

$$E_n = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 n^2 \qquad \text{and} \qquad E_n = \left(n + \frac{1}{2}\right)\hbar\omega_{\rm cl} \ ,$$

where $n = 1, 2, 3, \ldots$ for the infintie square well and $0, 1, 2, 3, \ldots$ for the simple harmonic oscillator, m is the particle mass, a is the well width, and $\omega_{\rm cl}$ simple harmonic oscillator frequency which enters the quantum mechanical description as parameter in the simple harmonic oscillator potential. What are the revival times for general wave functions for these two systems?

c) What are the classical revival times for a particle in a infinite square well system and in a simple harmonic oscillator system in terms of, respectively, energy and $\omega_{\rm cl}$? The classical times are just the oscillation periods for the particles. The particle in the infinite square well is assumed to be just bouncing between the walls without loss of kinetic energy.

d) For what classical energy E in units of E_1 (i.e., E/E_1) are the quantum mechanical and classical revival times equal for the infinite square well? What is the relationship between the quantum mechanical and classical revival times for the simple harmonic oscillator?

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003 qfull 01000 3 5 0 tough thinking: 3-d infinite cubical well
Extra keywords: (Gr-124:4.2), separation of Schrödinger equation

7. Consider an infinite cubical well or particle-in-a-box system. The potential is

$$V(x, y, x) = \begin{cases} 0, & \text{for } x,\ y, \text{ and } z \text{ in the range 0 to } a; \\ \infty, & \text{otherwise.} \end{cases}$$

The wave functions must be zero at the boundaries for an infinite well recall.

a) Solve for the stationary states from the 3-dimensional Schrödinger equation and find their energies in terms of quantum numbers n_x, n_y, and n_z. **HINTS:** Separate the Schrödinger equation into x, y, and z components. Identify the sum of the separation constants as energy or, if you prefer, energy times a constant. Solve separately matching the boundary conditions and then assemble the normalized **TOTAL SOLUTION**. Of course, all three dimensions behave the same so only one of them really needs to be done—which is **NOT** to say that each one is a total solution all by itself.

b) Is there energy degeneracy? Why?

c) Determine the 6 lowest energies and their degeneracy? **HINTS:** A systematic approach would be fix an $n_{\rm max} = \max(n_x, n_y, n_z)$ and count all energies and their degeneracies governed by that $n_{\rm max}$. One works one's way up from $n_{\rm max} = 1$ to as high as one needs to go to encompass the 6 lowest energies. Each $n_{\rm max}$ governs the energies between $n_{\rm max}^2 + 2$ and $3n_{\rm max}^2$ (where we have written the in dimensionless form). Note, e.g., that states described by $(n_x = 4, n_y = 1, n_z = 1)$, $(n_x = 1, n_y = 4, n_z = 1)$, and $(n_x = 1, n_y = 1, n_z = 4)$ are all distinct and degenerate.

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003 qfull 01100 1 3 0 easy math: pi-states of a benzene ring
Extra keywords: (Ha-323:2.1)

8. Imagine that we have 6 free electrons in 1-d circular system of radius $r = 1.53\,\text{Å}$. This system is a simple model of a benzene ring molecule (C_6H_6) of 6 carbon atoms each bonded to a hydrogen (Ke-153). The carbons are bonded by bonded by a single-double bond superposition. The free electron system on the benzene constitute the benzene *pi*-states.

a) Obtain expressions for the eigenstates, wavenumbers, and eigen-energies of the free electrons. Re-express the wavenumbers and energies in terms of Angstroms and electronvolts. Note $\hbar^2/(2m) = 3.81\,\text{eV-Å}^2$ for electrons. Sketch the energy level diagram.

b) One electron per carbon lies in the circular state for a benzene ring: these are the π electrons. Assuming that two electrons can be found in any state, what is the total energy of the ground state configurations? **NOTE:** Two electrons can be found in any state because there are two spin states they can be found in. Thus the Pauli exclusion principle is maintained: i.e., only one electron can be found in any single-particle state (e.g., Gr-180).

c) What is the energy difference in eV between the lowest empty level and highest occupied level for the ground state configuration? This is the radiation absorption threshold. What is the threshold line wavelength in microns? In what wavelength regime is this line? **NOTE:** The constant $hc = 1.23984\,\text{eV-}\mu\text{m}$.

d) Now imagine we broke the benzene ring, but magically kept the length constant. Obtain expressions for the eigenstates, wavenumbers, and eigen-energies of the free electrons. Re-express the wavenumbers and energies in terms of Angstroms and electronvolts. Sketch the energy levels on the previous energy level diagram.

e) What is the ground state energy for the broken ring. What is the change in ground state energy from the unbroken ring. This change is a contribution to the energy required to break the ring or the energy of a resonant π bond.

f) I know we said that somewhere that quantum mechanical bound states always had to have $E > V_{\text{min}}$. But in the ring case we had $V_{\text{min}} = 0$, and we have a state with $E = 0$. So why do we have this paradox? Is the paradox possible in 2 dimensions or 3 dimensions?

Chapt. 4 The Simple Harmonic Oscillator (SHO)

Multiple-Choice Problems

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004 qmult 00100 2 4 1 moderate deducto-memory: SHO eigen-energies

1. "Let's play *Jeopardy*! For \$100, the answer is: $\hbar\omega$.

   a) What is the energy difference between adjacent simple harmonic ocsillator energy levels, Alex?
   b) What is the energy difference between adjacent infinite square well energy levels, Alex?
   c) What is the energy difference between most adjacent infinite square well energy levels, Alex?
   d) What is the energy difference between the first two simple harmonic ocsillator energy levels **ONLY,** Alex?
   e) What is the bar where physicists hang out in Las Vegas, Alex?

Full-Answer Problems

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004 qfull 00100 2 3 0 moderate math: SHO ground state analyzed
Extra keywords: (Gr-19:1.14)

1. The simple harmonic oscillator (SHO) ground state is

$$\Psi_0(x,t) = Ae^{-\beta^2x^2/2-iE_0t/\hbar} \ ,$$

where

$$E_0 = \frac{\hbar\omega}{2} \qquad \text{and} \qquad \beta = \sqrt{\frac{m\omega}{\hbar}} \ .$$

   a) Verify that the wave function satisfies the full Schrödinger equation for the SHO. Recall that the SHO potential is $V(x) = (1/2)m\omega^2x^2$.

   b) Determine the normalization constant A.

   c) Calculate the expectation values of x, x^2, p, and p^2.

   d) Calculate σ_x and σ_p, and show that they satisfy the Heisenberg uncertainty principle.

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004 qfull 00200 2 3 0 moderate thinking: SHO classically forbidden
Extra keywords: (Gr-43:2.15) classical turning points

2. What is the probability is of finding a particle in the ground state of a simple harmonic oscillator potential outside of the classically allowed region: i.e., beyond the classical turning points? **HINT:** You will have to use a table of the integrated Gaussian function.

---

004 qfull 00300 2 5 0 moderate thinking: mixed SHO stationary states
Extra keywords: (Gr-43:2.17)

3. A particle in a simple harmonic oscillator (SHO) potential has initial wave function

$$\Psi(x,0) = A\left[\psi_0 + \psi_1\right] \ ,$$

where A is the normalization constant and the ψ_i are the standard form 0th and 1st SHO eigenstates. Recall the potential is

$$V(x) = \frac{1}{2}m\omega^2 x^2 \ .$$

Note ω is just an angular frequency parameter of the potential and not **NECESSARILY** the frequency of anything in particular. In the classical oscillator case ω is the frequency of oscillation, of course.

a) Determine A assuming it is pure real as we are always free to do.

b) Write down $\Psi(x,t)$. There is no need to express the ψ_i explicitly. Why must this $\Psi(x,t)$ be the solution?

c) Determine $|\Psi(x,t)|^2$ in simplified form. There should be a sinusoidal function of time in your simplified form.

d) Determine $\langle x\rangle$. Note that $\langle x\rangle$ oscillates in time. What is its angular frequency and amplitude.

e) Determine $\langle p\rangle$ the quick way using the 1st formula of Ehrenfest's theorem. Check that the 2nd formula of Ehrenfest's theorem holds.

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004 qfull 01000 3 5 0 tough thinking: infinite square well/SHO hybrid

Extra keywords: (Mo-424:9.4)

4. Say you have the potential

$$V(x) = \begin{cases} \infty \ , & x < 0; \\ \dfrac{1}{2}m\omega^2 x^2 & x \geq 0. \end{cases}$$

a) By reflecting on the nature of the potential **AND** on the boundary conditions, identify the set of Schrödinger equation eigenfunctions satisfy this potential. Justify your answer. **HINTS:** Don't try solving the Schrödinger equation directly, just use an already known set of eigenfunctions to identify the new set. This shouldn't take long.

b) What is the expression for the eigen-energies of your eigenfunctions?

c) What factor must multiply the already-known (and already normalized) eigenfunctions you used to construct the new set you found in part (a) in order to normalize the new eigenfunctions? **HINT:** Use the evenness or oddness (i.e., definite parity) of the already-known set.

d) Show that your new eigenfunctions are orthogonal. **HINT:** Use orthogonality and the definite parity of the already-known set.

e) Show that your eigenfunctions form a complete set given that the already-known set was complete. **HINTS:** Remember completeness only requires that you can expand any suitably well-behaved function (which means I think it has to be piecewise continuous (Ar-435) and square-integrable (CT-99) satisfying the same boundary conditions as the set used in the expansion. You don't have to be able to expand any function. Also, use the completeness of the already-known set.

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004 qfull 01100 3 5 0 tough thinking: Hermite polynomials 1

5. The generating function method is a powerful method for obtaining the eigenfunctions of Sturm-Liouville Hermitian operators and some of their general properties. One can possibly obtain with only moderately arduous labor some special values, the norm value, a general series formula for the eigenfunctions, and recurrence relations for iteratively constructing the complete set of eigenfunctions. The only problem is who the devil thought up the generating function?

   In the case of Hermite polynomials, the generating function—which may or may not have been thought up by French mathematician Charles Hermite (1822–1901)—is

$$g(x,t) = e^{-t^2+2tx} = \sum_{n=0}^{\infty} H_n \frac{t^n}{n!}$$

   (Ar-609ff; WA-644). The H_n are the Hermite polynomials: they are functions of x and n is their order.

   Actually, the **HERMITE EQUATION** needs a weight function e^{-x^2} to be put in Sturm-Liouville self-adjoint form (Ar-426, WA-486). Alternatively, the Hermite polynomials times $e^{-x^2/2}$ satisfy a Sturm-Liouville Hermitian operator equation which happens to be the time-independent Schrödinger equation for the 1-dimensional quantum mechanical simple harmonic oscillator (Ar-612, WA-638). The 1-dimensional quantum mechanical simple harmonic oscillator is one of those few quantum mechanical systems with an analytic solution.

   NOTE: The parts of this question are independent: i.e., you should be able to do any of the parts without having done the other parts.

   a) Find the 1st recurrence relation

$$H_{n+1} = 2xH_n - 2nH_{n-1}$$

   by differentiating both the generating function and its and series expansion with respect to t. This recurrence relation provides a means of finding any order of Hermite polynomial. **HINT:** You will need to re-index summations and make use of the uniqueness theorem of power series.

   b) Find the 2nd recurrence relation

$$H_n' = 2nH_{n-1}$$

   by differentiating both the generating function and its and series expansion with respect to x. **HINT:** You will need to re-index summations and make use of the uniqueness theorem of power series.

   c) Use the 1st recurrence relation to work out and tabulate the polynomials up to 3rd order: i.e., find H_0, H_1, H_2, and H_3. You can find the first two polynomials (i.e., the 0th and 1st order polynomials) needed to start the recurrence process by a simple Taylor's series expansion of generating function.

   d) Use the 1st recurrence relation to prove that the order of a Hermite polynomial agrees with its polynomial degree (which is the degree of its highest degree term) and that even order Hermite polynomials are even functions and the odd order ones are odd functions. The last result means that the Hermite polynomials have definite parity (i.e., are either even or odd functions). **HINT:** Use proof by induction and refer to collectively to the results to be proven as "the results to be proven". If you didn't get H_0 and H_1 explicitly in part (c), you can assume H_0 has degree 0 and H_1 has degree 1.

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004 qfull 01110 3 5 0 tough thinking: Hermite polynomials 2

6. Now for some more Hermite polynomial results. Recall the Hermite polynomial generating function is

$$g(x,t) = e^{-t^2+2tx} = \sum_{n=0}^{\infty} H_n \frac{t^n}{n!}$$

(Ar-609ff; WA-644). The H_n are the Hermite polynomials: they are functions of x and n is their order. Also recall the two recurrence relations

$$H_{n+1} = 2xH_n - 2nH_{n-1} \qquad \text{and} \qquad H'_n = 2nH_{n-1}$$

and the first few Hermite polynomials which are given in the table below.

Table: Hermite Polynomials

Order	Polynomial
0	$H_0 = 1$
1	$H_1 = 2x$
2	$H_2 = 4x^2 - 2$
3	$H_3 = 8x^3 - 12x$
4	$H_4 = 16x^4 - 48x^2 + 12$
5	$H_5 = 32x^5 - 160x^3 + 120x$
6	$H_6 = 64x^6 - 480x^4 + 720x^2 - 120$

NOTE: The parts of this question are largely independent: i.e., you should be able to do most parts without having done others.

a) Now for something challenging. Show that

$$g(x,t) = e^{-t^2+2tx} = \sum_{\ell=0}^{\infty} \frac{(-t^2+2tx)^\ell}{\ell!} = \sum_{n=0}^{\infty} \frac{t^n}{n!} \sum_{k=0}^{[n/2]} \frac{n!}{(n-2k)!k!}(-1)^k(2x)^{n-2k}$$

which implies that

$$H_n = \sum_{k=0}^{[n/2]} \frac{n!}{(n-2k)!k!}(-1)^k(2x)^{n-2k} \ .$$

Note

$$[n/2] = \begin{cases} n/2 & \text{for } n \text{ even;} \\ (n-1)/2 & \text{for } n \text{ odd.} \end{cases}$$

HINTS: You will have to expand $(-t^2+2tx)^n$ in a binomial series and then re-order the summation. A schematic table of the terms ordered in row by ℓ and in column by k makes the re-ordering of the summation clearer. One should add up diagonals rather than rows.

b) Prove the following special results from the generating function:

$$H_{2n}(0) = (-1)^n \frac{(2n)!}{n!} \ , \qquad H_{2n+1}(0) = 0 \ , \qquad H_n(x) = (-1)^n H_n(-x) \ .$$

The last results shows that the Hermite polynomials have definite parity: even for n even; odd for n odd.

c) What is called the Rodrigues's formula for the Hermite polynomials can also be derived from the generating function:

$$H_n = (-1)^n e^{x^2} \frac{\partial^n}{\partial x^n}(e^{-x^2}) \ .$$

Derive this formula. **HINTS:** Write

$$g(x,t) = e^{-t^2+2tx} = e^{x^2} e^{-(t-x)^2}$$

and note that

$$\frac{\partial f(t-x)}{\partial t} = -\frac{\partial f(t-x)}{\partial x} .$$

d) Now show that Hermite's differential equation

$$H_n'' - 2xH_n' + 2nH_n = 0$$

follows from the two recurrence relations. This result shows that the Hermite polynomials satisfy Hermite's differential equation.

e) Now consider the Hermite differential equation

$$h'' - 2xh' + 2\nu h = 0 ,$$

where ν is not necessarily an integer ≥ 0. Try a power series solution

$$h = \sum_{\ell=0}^{\infty} a_\ell x^\ell ,$$

and show for sufficiently large ℓ and x that the series solutions approximate growing exponentials of the form e^{x^2} and xe^{x^2}—unless ν is a positive or zero integer in which case one gets what kind of solution?

f) Hey this question is just going on and on. The Hermite differential equation cannot be written in an eigenproblem form with a Hermitian operator since the operator

$$\frac{\partial^2}{\partial x^2} - 2x\frac{\partial}{\partial x}$$

is not, in fact, Hermitian. I won't ask you to prove this since I don't what to do that myself tonight. But if you substitute for $H_n(x)$ (with n a positive or zero integer) the function

$$\psi_n(x)e^{x^2/2}$$

in the Hermite differential equation, you do an eigenproblem with a Hermitian operator. Find this eigenproblem equation. What are the eigenfunctions and eigenvalues? Are the eigenfunctions square-integrable: i.e., normalizable in a wave function sense? Do the eigenfunctions have definite parity? Are the eigenvalues degenerate for square-integrable solutions? Based on a property of eigenfunctions of a Hermitian operator what can you say about the orthogonality of the eigenfunctions?

g) In order to normalize the eigenfunctions of part (i) in a wave function sense consider the relation

$$\sum_{m,n=0}^{\infty} \frac{s^m}{m!}\frac{t^n}{n!}e^{-x^2}H_m H_n = e^{-x^2}g(x,s)g(x,t) = e^{-x^2}e^{-s^2+2sx}e^{-t^2+2tx} .$$

Integrate both sides over all x and use uniqueness of power series to find the normalization constants and incidently verify orthogonality.

h) Now here in part infinity we will make the connection to physics. The simple harmonic oscillator time independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial y^2} + \frac{1}{2}m\omega^2 y^2\psi = E\psi .$$

One can reduce this to the dimensionless eigenproblem of part (i), by changing the variable with

$$x = \beta y \ .$$

To find β, let

$$A = \frac{\hbar^2}{2m} \qquad \text{and} \qquad B = \frac{1}{2} m\omega^2$$

and divide equation through by an unknown C, equate what needs to be equated, and solve for C and β. What are the physical solutions and eigen-energies of the SHO eigenproblem?

i) Check to see if Charles Hermite (1822–1901) did think up the Hermite polynomial generating function at the St. Andrews MacTutor History of Mathematics Archive:

http://www-groups.dcs.st-and.ac.uk/~history/BiogIndex.html

HINTS: You don't have to do this in a test *mise en scène.*

Chapt. 5 Free Particles and Momemtum Representation

Multiple-Choice Problems

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005 qmult 00100 1 1 2 easy deducto-memory: definition free particle

1. A free particle is:

   a) bound. b) unbound. c) both bound and unbound.
   d) neither bound nor unbound. e) neither here nor there.

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005 qmult 00200 1 4 5 easy deducto-mem: free particle system

2. The free particle system is one with where the potential is:

   a) the simple harmonic oscillator potential (SHO). b) a quasi-SHO potential.
   c) an infinite square well potential. d) a finite square well potential.
   e) zero (or a constant) everywhere.

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005 qmult 00300 1 4 4 easy deducto-mem: free particle eigenfunction

3. The general expression for the free particle energy eigenfunction in 1-dimension is:

   a) e^{ikx}, where $k = \pm E$. b) e^{kx}, where $k = \pm E$. c) e^{kx}, where $k = \pm\sqrt{2mE/\hbar^2}$.
   d) e^{ikx}, where $k = \pm\sqrt{2mE/\hbar^2}$. e) e^{kx^2}, where $k = \pm\sqrt{2mE/\hbar^2}$.

---

005 qmult 00400 1 4 1 easy deducto-mem: free particle normalization 1

4. The free particle energy eigenfunctions are not physical states that a particle can actually be in because they:

   a) can't be normalized (i.e., they arn't square-integrable).
   b) can be normalized (i.e., they are square-integrable).
   c) are growing exponentials.
   d) don't exist.
   e) do exist.

---

005 qmult 00500 1 1 3 easy memory: free particle normalization 2

5. The free particle stationary states:

   a) can be occupied by a particle. b) can be occupied by two particles.
   c) cannot actually be occupied by a particle. d) are unknown.
   e) are normalizable.

Full-Answer Problems

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005 qfull 00100 2 5 0 easy thinking: momentum representation

Extra keywords: (Gr-49:2.21)

1. The initial wave function of a free particle is

$$\Psi(x,0) = \begin{cases} A\ , & x \in [-a,a]; \\ 0\ , & \text{otherwise,} \end{cases}$$

where a and A are positive real numbers. The particle is in a completely zero potential environment since it is a free particle.

a) Determine A from normalization.

b) Determine $\psi(k) = \Psi(k, 0)$ the time-zero wavenumber representation of the particle state. It is the Fourier transform of $\Psi(x, 0)$. What is $\Psi(k, t)$? Sketch $\psi(k)$. Locate the global maximum and the zeros of $\psi(k)$. Give the expression for the zeros (i.e., for the location of the zeros).

c) Determine the wavenumber space probability density $|\Psi(k, t)|^2$ and show then that $\Psi(k, t)$ is normalized in wavenumber space. (You can use a table integral.) Sketch $|\Psi(k, t)|^2$ and locate the global maximum and the zeros. Give the expression for the zeros.

d) Crudely estimate and then calculate exactly σ_x, σ_k, and σ_p for time zero. Are the results consistent with the Heisenberg uncertainty principle?

---

005 qfull 00200 3 3 0 tough math: k-representation of half exponential

Extra keywords: (Mo-140:4.4)

2. At time zero, a wave function for a free particle in a zero-potential 1-dimensional space is:

$$\Psi(x, 0) = A e^{-|x|/\ell} e^{ik_0 x} .$$

a) Determine the normalization constant A. **HINT:** Remember it's $\Psi(x, 0)^* \Psi(x, 0)$ that appears in the normalization equation.

b) Sketch the x-space probability density $|\Psi(x, 0)|^2$. What is the e-folding distance of the probability density?

NOTE: The e-folding distance is a newish term that means the distance in which an exponential function changes by a factor of e. It can be generalized to any function $f(x)$ using the formula

$$x_e = \left| \frac{f(x)}{f(x)'} \right| ,$$

where x_e is the generalized e-folding distance. The generalized e-folding distance is only locally valid to the region near the x where the functions are evaluated. The generalized e-folding distance is also sometimes called the scale height. If $f(x)$ were an exponential function, x_e would be the e-folding distance in the narrow sense. If $f(x)$ were a linear function, x_e would be the distance to the zero of the function.

c) Show that the wavenumber representation of free particle state is

$$\Psi(k) = \sqrt{\frac{2\ell}{\pi}} \frac{1}{1 + (k_0 - k)^2 \ell^2} .$$

This, of course, is the Fourier transform of $\Psi(x, 0)$. Recall the wavenumber representation is time-independent since the wavenumber eigenstates are the stationary states of the potential.

d) Confirm that $\Psi(k)$ is normalized in wavenumber space. **HINTS:** You will probably need an integral table—unless you're very, very good. Also remember it's $\Psi(k)^* \Psi(k)$ that appears in the normalization integral; always easy to forget this when dealing with pure real functions.

e) Write down the time-dependent solution $\Psi(x, t)$ in Fourier transform form? Don't try to evaluate the integral. What is ω in terms of k and energy E?

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005 qfull 00300 3 3 0 tough math: Gaussian free wave packet spreading

Extra keywords: (Gr-50:2.22)

3. A free particle has an initial Gaussian wave function

$$\Psi(x,0)=Ae^{-ax^2}\ ,$$

where a and A are real positive constants.

a) Normalize $\Psi(x,0)$. **HINT:** Recall that the integrand is $|\Psi(x,t)|^2=\Psi(x,t)^*\Psi(x,t)$. I'm always forgetting this myself when the function is pure real and there is no imaginary part to remind me of it.

b) Determine the wavenumber representation $\Psi(k)$ (which is time-independent). This involves a Gaussian integral where you have to complete the square in an exponential exponent. Note

$$\begin{aligned}\exp[-(ax^2+bx)]&=\exp\left[-a\left(x^2+\frac{b}{a}x+\frac{b^2}{4a^2}\right)\right]\exp\left(\frac{b^2}{4a^2}\right)\\&=\exp\left[-a\left(x+\frac{b}{2a}\right)^2\right]\exp\left(\frac{b^2}{4a}\right)\ .\end{aligned}$$

The exponetial factor $\exp\left(b^2/4a\right)$ comes out of the integral and the integral over the whole x-axis is just a simple Gaussian integral.

c) Determine $\Psi(x,t)$. You have to again do a Gaussian integral where you have to complete the square in an exponential exponent. It's not that hard to do, but it is tedious and small errors can mess things up.

d) Find the probability density $|\Psi(x,t)|^2$. This should be a Gaussian if all goes well. Sketch the function and identify the standard deviation σ. What happens to the probability density with time. **HINT:** Note the identities

$$\begin{aligned}\left[\exp\left(\frac{a+ib}{c+id}\right)\right]^*&=\left\{\exp\left[\frac{ac+i(bc-ad)+bd}{c^2+d^2}\right]\right\}^*\\&=\left\{\exp\left[\frac{ac-i(bc-ad)+bd}{c^2+d^2}\right]\right\}\\&=\left[\exp\left(\frac{a-ib}{c-id}\right)\right]\end{aligned}$$

and

$$\left(\sqrt{a+ib}\right)^*=\left(\sqrt{re^{i\phi}}\right)^*=\left(\sqrt{r}e^{i\phi/2}\right)^*=\sqrt{r}e^{-i\phi/2}\ ,$$

where $a+ib$ magnitude and phase are $r=\sqrt{a^2+b^2}$ and $\phi=\tan^{-1}(b/a)$, respectively.

e) Find $\langle x\rangle$, $\langle x^2\rangle$, σ_x, $\langle p\rangle$, $\langle p^2\rangle$, and σ_p. **HINT:** These results follow immediately from the Gaussian nature of the functions in parts (d) and (b).

f) Check that the Heisenberg uncertainty principle is satisfied. Does the equality ever hold? What's true about the wave function at the time when the equality holds that is not true at other times?

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005 qfull 00400 3 5 0 tough thinking: general free wave packet spreading

Extra keywords: (CT-342:4)

4. Consider a free particle in one dimension.

a) Show using Ehrenfest's theorem that $\langle x\rangle$ is linear in time and that $\langle p\rangle$ is constant.

b) Write the equation of motion (time evolution equation) for $\langle p^2\rangle$, then $\langle [x,p]_+\rangle$ (the subscript $+$ indicates anticommutator), and then $\langle x^2\rangle$: i.e., obtain expressions for the time derivatives of these quantities. Simplify the expressions for the derivatives as much as possible, but without loss of generality. You should get nice compact formal results. Integrate these derivatives with respect to time and remember constants of integration.

c) Using the results obtained in parts (a) and (b) and for suitable choice of one of the constants of integration, show that

$$\left(\Delta x^2\right)(t) = \frac{1}{m^2}\left(\Delta p^2\right)_0 t^2 + \left(\Delta x^2\right)_0$$

where $\left(\Delta x^2\right)_0$ and $\left(\Delta p^2\right)_0$ are the initial standard deviations.

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005 qfull 00500 2 5 0 moderate thinking: x-op and k-op in x and k representation

5. For a free particle in one dimension, the position and wavenumber representations of the state expanded in eigenfunctions of the other representation, are, respectively:

$$\Psi(x,t) = \int_{-\infty}^{\infty} \phi(k,t)\frac{e^{ikx}}{\sqrt{2\pi}}\,dk = \int_{-\infty}^{\infty} \phi(k)\frac{e^{i(kx-\omega t)}}{\sqrt{2\pi}}\,dk$$

and

$$\Phi(k,t) = \phi(k)e^{-i\omega t} = \left[\int_{-\infty}^{\infty} \Psi(x,0)\frac{e^{-ikx}}{\sqrt{2\pi}}\,dx\right] e^{-i\omega t} \ ,$$

where

$$\omega = \frac{\hbar k^2}{2m} \ .$$

a) The expectation value for a general observable in Q the position representation is

$$\langle Q\rangle = \int_{-\infty}^{\infty} \Psi(x,t)^* Q \Psi(x,t)\,dx \ ,$$

where Q can depend on x and differentiations with respect to x, but not on k nor differentiations with respect to k. Substitute for $\Psi(x,t)$ using the wavenumber expansion and find an expression that is a triple integral.

b) The wavenumber observable in the position representation is

$$k_{\rm op} = \frac{1}{\hbar}p_{\rm op} = \frac{1}{i}\frac{\partial}{\partial x} \ ,$$

where $p_{\rm op}$ is the momentum observable in the position representation. Using the result of the part (a) answer, identify the wavenumber observable in the wavenumber representation.

c) The position observable $x_{\rm op}$ in the position representation is just the coordinate x. Using the result of the part (a) answer, identify the position observable in the wavenumber representation.

---

005 qfull 00510 3 5 0 tough thinking: x-op and p-op in x and p representation

Extra keywords: (Gr-117:3.51) a very general solution is given

6. In the position representation, the position operator $x_{\rm op}$ is just x, a multiplicative variable. The momentum operator $p_{\rm op}$ in the position representation is

$$p_{\rm dif} = \frac{\hbar}{i}\frac{\partial}{\partial x} \ .$$

where we use the subsript "dif" here to indicate explicitly that this is a differentiating operator.

a) Find the momentum operator $p_{\rm op}$ in the momentum representation. **HINTS:** Operate with $p_{\rm dif}$ on the Fourier transform expansion of a general wave function

$$\Psi(x,t)=\int_{-\infty}^{\infty}\Psi(p,t)\frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}\,dp$$

and work the components of the integral around (using whatever tricks you need) until you have

$$p_{\rm dif}\Psi(x,t)=\int_{-\infty}^{\infty}f(p,t)\frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}\,dp\ .$$

The function $f(p,t)$ is the Fourier transform of $p_{\rm dif}\Psi(x,t)$ and operator acting on $\Psi(p,t)$ to give you $f(p,t)$ is the momentum operator in the momentum representation.

b) Find the position operator $x_{\rm op}$ in the momentum representation. **HINTS:** The same as for part (a), *mutatis mutandis*: find the Fourier transform of wave function $x\Psi(x,t)$, etc.

c) What are the momentum representation versions of x^k and $p_{\rm dif}^\ell$?

d) What is the momentum representation versions of $x^k p_{\rm dif}^\ell$ and $p_{\rm dif}^\ell x^k$. By the by, you should remember how to interpret $x^k p_{\rm dif}^\ell$ and $p_{\rm dif}^\ell x^k$: they are two successive operators acting on understood function to the right. Explicitly for a general function $f(x)$, one could write

$$x^k p_{\rm dif}^\ell f(x)=x^k\left[p_{\rm dif}^\ell f(x)\right]$$

and

$$p_{\rm dif}^\ell x^k f(x)=p_{\rm dif}^\ell\left[x^k f(x)\right]\ ,$$

Unfortunately, there is sometimes ambiguity in writing formulae with operators: try to be clear.

e) What is the momentum representation version of $Q(x,p_{\rm dif})$ where Q is any linear combination of powers of x and $p_{\rm dif}$ including mixed powers. **HINTS:** Consider the general term

$$\ldots x^k p_{\rm dif}^\ell x^m p_{\rm dif}^n$$

and figure out what commutes with what.

f) Show that the expectation value of Q is the same in both representations. **HINT:** Remember the Dirac delta function

$$\delta(k-k')=\int_{-\infty}^{\infty}\frac{e^{i(k-k')x}}{2\pi}\,dx\ .$$

Chapt. 6 Foray into Advanced Classical Mechanics

Multiple-Choice Problems

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006 qmult 00100 1 1 2 easy memory: Newton's 2nd law

1. Classical mechanics can be very briefly summarized by:

    a) Newton's *Principia*.
    b) Newton's 2nd law.
    c) Lagrange's *Traité de mécanique analytique*.
    d) Euler's 80 volumes of mathematical works.
    e) Goldstein 3rd edition.

---

006 qmult 00200 1 4 1 easy deducto-memory: Lagrangian formulation
Extra keywords: see GPS-12, 17, and 48

2. "Let's play *Jeopardy*! For \$100, the answer is: A formulation of classical mechanics that is usually restricted to systems with holonomic or semi-holonomic virtual-displacement workless constraints without dissipation and uses the function $L = T - V$."

    a) What is the Lagrangian formulation, Alex?
    b) What is the Hamiltonian formulation, Alex?
    c) What is the Leibundgutian formulation, Alex?
    d) What is the Harrisonian formulation, Alex?
    e) What is the Sergeant Schultzian formulation, Alex?

---

006 qmult 00300 1 1 5 easy memory: Hamilton's principle

3. A fruitful starting point for the derivation of Lagrange's equations is:

    a) Lagrange's lemma.
    b) Newton's scholium.
    c) Euler's conjecture.
    d) Laplace's hypothesis
    e) Hamilton's principle.

Full-Answer Problems

---

006 qfull 01000 2 5 0 moderate thinking: Lorentz force

1. The Lorentz force

$$\vec{F} = q\left(\vec{E} + \frac{\vec{v}}{c} \times \vec{B}\right)$$

(here expressed in Gaussian units: Ja-238) can be obtained from Lagrange's equations using a Lagrangian containing a generalized potential

$$U = q\left(\phi - \frac{\vec{v}}{c} \cdot \vec{A}\right) \ ,$$

where ϕ is the electric potential and $\vec{A}$ is the vector potential of electromagnetism. The Lagrangian is $L = T - U$, where T is the kinetic energy. Lagrange's equations are

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0 \ ,$$

where q_i is a generalized coordinate (not charge) and $\dot{q}_i$ is the total time derivative of q: (i.e., the rate of change of q_i which describes an actual particle.

Work from the Lorentz force expression for component i to

$$F_i = -\frac{\partial U}{\partial x_i} + \frac{d}{dt}\left(\frac{\partial U}{\partial \dot{x}_i}\right) \ ,$$

where the x_i are the Cartesian coordinates of a particle ($\dot{x}_i$ are the particle velocity components). Then verify that

$$m\ddot{x}_i = F_i$$

follows from the Lagrange equations.

You may need some hints. Recall that

$$\vec{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t} \qquad \text{and} \qquad B = \nabla \times \vec{A}$$

(Ja-219). The Levi-Civita symbol ε_{ijk} will be useful since

$$(\nabla \times A)_i = \varepsilon_{ijk}\frac{\partial}{\partial x_j}A_k \ .$$

where Einstein summation has been used. Recall

$$\varepsilon_{ijk} = \begin{cases} 1, & ijk \text{ cyclic;} \\ -1, & ijk \text{ anticyclic;} \\ 0, & \text{if two indices the same.} \end{cases}$$

The identity (with Einstein summation)

$$\varepsilon_{ijk}\varepsilon_{i\ell m} = \delta_{j\ell}\delta_{km} - \delta_{jm}\delta_{k\ell}$$

is also useful. I've never found an elegant derivation of this last identity: the only proof seems to be by exhaustion. Note also that the total time derivative is interpreted as the rate of change of a quantity as the particle moves. Thus

$$\frac{dA_i}{dt} = \frac{\partial A_i}{\partial t} + \frac{\partial A_i}{\partial x_j}\frac{dx_j}{dt} = \frac{\partial A_i}{\partial t} + \frac{\partial A_i}{\partial x_j}\dot{x}_j = \frac{\partial A_i}{\partial t} + \frac{\partial A_i}{\partial x_j}v_j \ ,$$

where we again use Einstein summation.

Chapt. 7 Linear Algebra

Multiple-Choice Problems

---

007 qmult 00100 1 1 5 easy memory: vector addition

1. The sum of two vectors belonging to a vector space is:

    a) a scalar.
    b) another vector, but in a different vector space.
    c) a generalized cosine.
    d) the Schwarz inequality.
    e) another vector in the same vector space.

---

007 qmult 00200 1 4 4 easy deducto-memory: Schwarz inequality

2. "Let's play *Jeopardy*! For \$100, the answer is: $|\langle\alpha|\beta\rangle|^2 \leq \langle\alpha|\alpha\rangle\langle\beta|\beta\rangle$."

    What is ____________, Alex?

    a) the triangle inequality b) the Heisenberg uncertainty principle
    c) Fermat's last theorem d) the Schwarz inequality
    e) Schubert's unfinished last symphony

---

007 qmult 00300 1 4 5 easy deducto-memory: Gram-Schmidt procedure

3. Any set of linearly independent vectors can be orthonormalized by the:

    a) Pound-Smith procedure. b) Li Po tao. c) Sobolev method.
    d) Sobolev-P method. e) Gram-Schmidt procedure.

---

007 qmult 00400 1 4 4 moderate memory: definition unitary matrix

4. A unitary matrix is defined by the expression:

    a) $U = U^T$, where superscript T means transpose. b) $U = U^\dagger$. c) $U = U^*$.
    d) $U^{-1} = U^\dagger$. e) $U^{-1} = U^*$.

---

007 qmult 00500 2 3 4 moderate math: trivial eigenvalue problem

5. What are the eigenvalues of

$$\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \; ?$$

    a) Both are 0. b) 0 and 1. c) 0 and -1. d) 0 and 2. e) $-i$ and 1.

---

007 qmult 00600 1 4 5 moderate memory: riddle Hermitian matrix

6. Holy peccant poets Batman, it's the Riddler.

    I charge to the right and hit on a ket,
    and if it's not eigen, it's still in the set,
    I charge to left and with a quick draw
    make a new bra from out of a bra.

    Not fish nor fowl nor quadratic,
    not uncanny tho oft Q-mechanic,

and transposed I'm just the right me
if also complexicated as you can see.

My arrows down drawn from quivered,
the same when sped to the world delivered
aside from a steady factor, rock of reality,
mayhap of a quantum and that's energy.

a) A unitary operator.
b) A ket—no, no, a bra vector.
c) An eigenvalue.
d) Hamlet.
e) A Hermitian matrix.

Full-Answer Problems

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007 qfull 00090 1 5 0 easy thinking: ordinary vector space
Extra keywords: (Gr-77:3.1)

1. Consider ordinary 3-dimensional vectors with complex components specified by a 3-tuple: (x, y, z). They constitute a 3-dimensional vector space. Are the following subsets of this vector space vector spaces? If so, what is their dimension? **HINT:** See Gr-435 for all the properties a vector space must have.

   a) The subset of all vectors $(x, y, 0)$.

   b) The subset of all vectors $(x, y, 1)$.

   c) The subset of all vectors of the form (a, a, a), where a is any complex number.

---

007 qfull 00100 2 5 0 moderate thinking: vector space, polynomial
Extra keywords: (Gr-78:3.2)

2. A vector space is constituted by a set of vectors $\{|\alpha\rangle, |\beta\rangle, |\gamma\rangle, \ldots\}$ and a set of scalars $\{a, b, c, \ldots\}$ (ordinary complex numbers is all that quantum mechanics requires) subject to two operations vector addition and scalar multiplication obeying the certain rules. Note it is the relations between vectors that make them constitute a vector space. What they "are" we leave general. The rules are:

   i) A sum of vectors is a vector:
   $$|\alpha\rangle + |\beta\rangle = |\gamma\rangle \ ,$$
   where $|\alpha\rangle$ and $|\beta\rangle$ are any vectors in the space and $|\gamma\rangle$ also in the space. Note we have not defined what vector addition consists of. That definition goes beyond the general requirements.

   ii) Vector addition is commutative:
   $$|\alpha\rangle + |\beta\rangle = |\beta\rangle + |\alpha\rangle \ .$$

   iii) Vector addition is associative:
   $$(|\alpha\rangle + |\beta\rangle) + |\gamma\rangle = |\alpha\rangle + (|\beta\rangle + |\gamma\rangle) \ .$$

   iv) There is a zero or null vector $|0\rangle$ such that
   $$|\alpha\rangle + |0\rangle = |\alpha\rangle \ ,$$

v) For every vector $|\alpha\rangle$ there is an inverse vector $|-\alpha\rangle$ such that

$$|\alpha\rangle + |-\alpha\rangle = |0\rangle \ .$$

vi) Scalar multiplication of a vector gives a vector:

$$a|\alpha\rangle = |\beta\rangle \ .$$

vii) Scalar multiplication is distributive on vector addition:

$$a(|\alpha\rangle + |\beta\rangle) = a|\alpha\rangle + a(|\beta\rangle) \ .$$

viii) Scalar multiplication is distributive on scalar addition:

$$(a+b)|\alpha\rangle = a|\alpha\rangle + b|\alpha\rangle \ .$$

ix) Scalar multiplication is associative with respect to scalar multiplication:

$$(ab)|\alpha\rangle = a(b|\alpha\rangle) \ .$$

x) One has

$$0|\alpha\rangle = |0\rangle \ .$$

xi) Finally, one has

$$1|\alpha\rangle = |\alpha\rangle \ .$$

NOTE: Note that

$$|0\rangle = 0|\alpha\rangle = [1 + (-1)]|\alpha\rangle = |\alpha\rangle + (-1)|\alpha\rangle \ ,$$

and thus we find that

$$|-\alpha\rangle = -|\alpha\rangle \ .$$

So the subtraction of a vector is just the addition of its inverse. This is consistent with all ordinary math.

If any vector in the space can be written as linear combination of a set of linearly independent vectors, that set is called a basis and is said to span the set. The number of vectors in the basis is the dimension of the space. In general there will be infinitely many bases for a space.

Finally the question. Consider the set of polynomials $\{P(x)\}$ (with complex coefficients) and degree less than n. For each of the subsets of this set (specified below) answer the following questions: 1) Is the subset a vector space? Inspection usually suffices to answer this question. 2) If not, what property does it lack? 3) If yes, what is the most obvious basis and what is the dimension of the space?

a) The subset that is the whole set.

b) The subset of even polynomials.

c) The subset where the highest term has coefficient a (i.e., the leading coefficient is a) and a is a general complex number, except $a \neq 0$.

d) The subset where $P(x = g) = 0$ where g is a general real number. (To be really clear, I mean the subset of polynomials that are equal to zero at the point $x = g$.)

e) The subset where $P(x = g) = h$ where g is a general real number and h is a general complex number, except $h \neq 0$.

---

007 qfull 00110 2 5 0 moderate thinking: unique expansion in basis

Extra keywords: (Gr-78:3.3)

3. Prove that the expansion of a vector in terms of some basis is unique: i.e., the set of expansion coefficients for the vector is unique.

---

007 qfull 00200 3 5 0 tough thinking: Gram-Schmidt orthonormalization

Extra keywords: (Gr-79:3.4)

4. Say $\{|\alpha_i\rangle\}$ is a basis (i.e., a set of linearly independent vectors that span a vector space), but it is not orthonormal. The first step of the Gram-Schmidt orthogonalization procedure is to normalize the (nominally) first vector to create a new first vector for a new orthonormal basis:

$$|\alpha_1'\rangle = \frac{|\alpha_1\rangle}{||\alpha_1||} \ ,$$

where recall that the norm of a vector $|\alpha\rangle$ is given by

$$||\alpha|| = || \ |\alpha_1\rangle \ || = \sqrt{\langle\alpha|\alpha\rangle} \ .$$

The second step is create a new second vector that is orthogonal to the new first vector using the old second vector and the new first vector:

$$|\alpha_2'\rangle = \frac{|\alpha_2\rangle - |\alpha_1'\rangle\langle\alpha_1'|\alpha_2\rangle}{|| \ |\alpha_2\rangle - |\alpha_1'\rangle\langle\alpha_1'|\alpha_2\rangle \ ||} \ .$$

Note we have subtracted the projection of $|\alpha_2\rangle$ on $|\alpha_1'\rangle$ from $|\alpha_2\rangle$ and normalized.

a) Write down the general step of the Gram-Schmidt procedure.

b) Why must an orthonormal set of non-null vectors be a linearly independent.

c) Is the result of a Gram-Schmidt procedure independent of the order the original vectors are used? **HINT:** Say you first use vector $|\alpha_a\rangle$ of the old set in the procedure. The first new vector is just $|\alpha_a\rangle$ normalized: i.e., $|\alpha_a'\rangle = |\alpha_a\rangle/||\alpha_a||$. All the other new vectors will be orthogonal to $|\alpha_a'\rangle$. But what if you started with $|\alpha_b\rangle$ which in general is not orthogonal to $|\alpha_a\rangle$?

d) How many orthonormalized bases can an n dimensional space have in general? (Ignore the strange $n = 1$ case.) **HINT:** Can't the Gram-Schmidt procedure be started with any vector at all in the vector space?

e) What happens in the procedure if the original vector set $\{|\alpha_i\rangle\}$ does not, in fact, consist of all linearly independent vectors? To understand this case analyze another apparently different case. In this other case you start the Gram-Schmidt procedure with n original vectors. Along the way the procedure yields null vectors for the new basis. Nothing can be done with the null vectors: they can't be part of a basis or normalized. So you just put those null vectors and the vectors they were meant to replace aside and continue with the procedure. Say you got m null vectors in the procedure and so ended up with $n - m$ non-null orthonormalized vectors. Are these $n - m$ new vectors independent? How many of the old vectors were used in constructing the new $n - m$ non-null vectors and which old vectors were they? Can all the old vectors be recontructed from the the new $n-m$ non-null vectors? Now answer the original question.

f) If the original set did consist of n linearly independent vectors, why must the new orthonormal set consist of n linearly independent vectors? **HINT:** Should be just a corollary of the part (e) answer.

g) Orthonormalize the 3-space basis consisting of

$$|\alpha_1\rangle = \begin{pmatrix} 1+i \\ 1 \\ i \end{pmatrix}, |\alpha_2\rangle = \begin{pmatrix} i \\ 3 \\ 1 \end{pmatrix}, \quad \text{and} \quad |\alpha_3\rangle = \begin{pmatrix} 0 \\ 32 \\ 0 \end{pmatrix} .$$

Input the vectors into the procedure in the reverse of their nominal order: why might a marker insist on this? Note setting kets equal to columns is a lousy notation, but you-all know what I mean. The bras, of course, should be "equated" to the row vectors. **HINT:** Make sure you use the normalized new vectors in the construction procedure.

---

007 qfull 00300 2 3 0 moderate math: prove the Schwarz inequality

Extra keywords: (Gr-80:3.5)

5. As Andy Rooney says (or used to say if this problem has reached the stage where only old fogies remember that king of the old fogies) don't you just hate magic proofs where you start from some unmotivated expression and do a number of unmotivated steps to arrive at a result that you could never have been guessed from the way you were going about getting it. Well sans too many absurd steps, let us see if we can prove the Schwarz inequality

$$|\langle\alpha|\beta\rangle|^2 \leq \langle\alpha|\alpha\rangle\langle\beta|\beta\rangle$$

for general vectors $|\alpha\rangle$ and $|\beta\rangle$. Note the equality only holds in two cases. First when $|\beta\rangle = a|\alpha\rangle$, where a is some complex constant. Second, when either or both of $|\alpha\rangle$ and $|\beta\rangle$ are null vectors: in this case, one has zero equals zero.

NOTE: A few facts to remember about general vectors and inner products. Say $|\alpha\rangle$ and $|\beta\rangle$ are general vectors. By the definition of the inner product, we have that $\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*$. This implies that $\langle\alpha|\alpha\rangle$ is pure real. If c is a general complex number, then the inner product of $|\alpha\rangle$ and $c|\beta\rangle$ is $\langle\alpha|c|\beta\rangle = c\langle\alpha|\beta\rangle$. Next we note that that another inner-product property is that $\langle\alpha|\alpha\rangle \geq 0$ and the equality only holds if $|\alpha\rangle$ is the null vector. The norm of $|\alpha\rangle$ is $||\alpha|| = \sqrt{\langle\alpha|\alpha\rangle}$ and $|\alpha\rangle$ can be normalized if it is not null: i.e., for $|\alpha\rangle$ not null, the normalized version is $|\hat{\alpha}\rangle = |\alpha\rangle/||\alpha||$.

a) In doing the proof of the Schwarz inequality, it is convenient to have the result that the bra corresponding to $c|\beta\rangle$ (where $|\beta\rangle$ is a general vector and c is a general complex number) is $\langle\beta|c^*$. Prove this correspondance. **HINT:** Consider general vector $|\alpha\rangle$ and the inner product

$$\langle\alpha|c|\beta\rangle$$

and work your way by valid steps to

$$\langle\beta|c^*|\alpha\rangle^*$$

and that completes the proof since

$$\langle\alpha|\gamma\rangle = \langle\gamma|\alpha\rangle^*$$

for general vectors $|\alpha\rangle$ and $|\gamma\rangle$.

b) The next thing to do is to figure out what the Schwarz inequality is saying about vectors including those 3-dimensional things we have always called vectors. Let us a restrict the generality of $|\alpha\rangle$ by demanding it not be a null vector for which the Schwarz inequality is already proven. Since $|\alpha\rangle$ is not null, it can be normalized. Let $|\hat{\alpha}\rangle = |\alpha\rangle/||\alpha||$ be the normalized version of $|\alpha\rangle$. Divide the Schwarz inequality by $||\alpha||^2$. Now note that the component of $|\beta\rangle$ along the $|\hat{\alpha}\rangle$ direction is

$$|\beta_{||}\rangle = |\hat{\alpha}\rangle\langle\hat{\alpha}|\beta\rangle .$$

Evaluate $\langle\beta_{||}|\beta_{||}\rangle$. Now what is the Schwarz inequality telling us.

c) The vector component of $|\beta\rangle$ that is orthogonal to $|\hat{\alpha}\rangle$ (and therefore $|\beta_{||}\rangle$) is

$$|\beta_\perp\rangle = |\beta\rangle - |\beta_{||}\rangle \ .$$

Prove this and then prove the Schwarz inquality itself (for $|\alpha\rangle$ not null) by evaluating $\langle\beta|\beta\rangle$ expanded in components. What if $|\alpha\rangle$ is a null vector?

---

007 qfull 00310 1 3 0 easy math: find a generalized angle

Extra keywords: (Gr-80:3.6)

6. The general inner-product vector space definition of generalized angle according to Gr-440 is

$$\cos\theta_{\text{gen}} = \frac{|\langle\alpha|\beta\rangle|}{\sqrt{\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle}} \ ,$$

where $|\alpha\rangle$ and $|\beta\rangle$ are general non-zero vectors.

a) Is this definition completely consistent with the ordinary definition of an angle from the ordinary vector dot product? Why or why not?

b) Find the generalized angle between vectors

$$|\alpha\rangle = \begin{pmatrix} 1+i \\ 1 \\ i \end{pmatrix} \qquad \text{and} \qquad |\beta\rangle = \begin{pmatrix} 4-i \\ 0 \\ 2-2i \end{pmatrix} \ .$$

---

007 qfull 00400 1 3 0 easy math: prove triangle inequality

Extra keywords: (Gr-80:3.7)

7. Prove the triangle inequality:

$$||(|\alpha\rangle + |\beta\rangle)|| \leq ||\alpha|| + ||\beta|| \ .$$

HINT: Start with $||(|\alpha\rangle + |\beta\rangle)||^2$, expand, and use reality and the Schwarz inequality

$$|\langle\alpha|\beta\rangle|^2 \leq \langle\alpha|\alpha\rangle\langle\beta|\beta\rangle = ||\alpha||^2 \times ||\beta||^2 \ .$$

---

007 qfull 00500 3 3 0 tough math: simple matrix identities

Extra keywords: (Gr-87:3.12)

8. Prove the following matrix identities:

a) $(AB)^{\mathrm{T}} = B^{\mathrm{T}}A^{\mathrm{T}}$, where superscript "T" means transpose.

b) $(AB)^\dagger = B^\dagger A^\dagger$, where superscript † means Hermitian conjugate.

c) $(AB)^{-1} = B^{-1}A^{-1}$.

d) $(UV)^{-1} = (UV)^\dagger$ (i.e., UV is unitary) given that U and V are unitary. In other words, prove the product of unitary matrices is unitiary.

e) $(AB)^\dagger = AB$ (i.e., AB is Hermitian) given that A and B are commuting Hermitian matrices. Does the converse hold: i.e., does $(AB)^\dagger = AB$ imply A and B are commuting Hermitian matrices? **HINTS:** Find a trivial counterexample. Try $B = A^{-1}$.

f) $(A+B)^\dagger = A+B$ (i.e., $A+B$ is Hermitian) given that A and B are Hermitian. Does the converse hold? **HINT:** Find a trivial counterexample to the converse.

g) $(U+V)^\dagger = (U+V)^{-1}$ (i.e., $U+V$ is unitary) given that U and V are unitary—that is, prove this relation if it's indeed true—if it's not true, prove that it's not true. **HINT:** Find a simple counterexample: e.g., two 2×2 unit matrices.

---

007 qfull 00510 2 5 0 moderate thinking: commuting operations

Extra keywords: (Gr-84)

9. There are 4 simple operations that can be done to a matrix: inversing, (-1), complex conjugating $(*)$, transposing (T), and Hermitian conjugating $(\dagger)$. Prove that all these operations mutually commute. Do this systematically: there are

$$\binom{4}{2} = \frac{4!}{2!(4-2)!} = 6$$

combinations of the 2 operations. We assume the matrices have inverses for the proofs involving them.

---

007 qfull 00600 3 3 0 tough math: basis change results

Extra keywords: (Gr-87:3.14)

10. Do the following.

a) Prove that matrix multiplication is preserved under similarity or linear basis change: i.e., if $A_e B_e = C_e$ in the e-basis, then $A_f B_f = C_f$ in the f-basis where S is the basis change matrix from e-basis to the f-basis. Basis change does not in general preserve symmetry, reality, or Hermiticity. But since I don't want to find the counterexamples, I won't ask you to.

b) If H_e in the e-basis is a Hermitian matrix and the basis change to the f-basis U is unitary, prove that H_f is Hermitian: i.e., Hermiticity is is preserved.

c) Prove that basis orthonormality is preserved through a basis change U iff (if and only if) U is unitary.

---

007 qfull 00700 2 5 0 moderate thinking: square-integrable, inner product

Extra keywords: no analog Griffiths's problem, but discussion Gr-95–6, Gr2005-94–95

11. If $f(x)$ and $g(x)$ are square-integrable complex functions, then the inner product

$$\langle f|g\rangle = \int_{-\infty}^{\infty} f^* g\,dx$$

exists: i.e., is convergent to a finite value. In other words, that $f(x)$ are $g(x)$ are square-integrable is sufficient for the inner product's existence.

a) Prove the statement for the case where $f(x)$ and $g(x)$ are real functions. **HINT:** In doing this it helps to define a function

$$h(x) = \begin{cases} f(x) & \text{where } |f(x)| \geq |g(x)| \text{ (which we call the } f \text{ region);} \\ g(x) & \text{where } |f(x)| < |g(x)| \text{ (which we call the } g \text{ region),} \end{cases}$$

and show that it must be square-integrable. Then "squeeze" $\langle f|g\rangle$.

b) Now prove the statement for complex $f(x)$ and $g(x)$. **HINTS:** Rewrite the functions in terms of their real and imaginary parts: i.e.,

$$f(x) = f_{\text{Re}}(x) + i f_{\text{Im}}(x)$$

and

$$g(x) = g_{\text{Re}}(x) + i g_{\text{Im}}(x)\ .$$

Now expand

$$\langle f|g\rangle = \int_{-\infty}^{\infty} f^* g\,dx$$

in the terms of the new real and imaginary parts and reduce the problem to the part (a) problem.

c) Now for the easy part. Prove the converse of the statement is false. **HINT:** Find some trivial counterexample.

d) Now another easy part. Say you have a vector space of functions $\{f_i\}$ with inner product defined by

$$\int_{-\infty}^{\infty} f_j^* f_k\,dx \ .$$

Prove the following two statements are equivalent: 1) the inner product property holds; 2) the functions are square-integrable.

---

007 qfull 00800 2 3 0 moderate math: Gram-Schmidt, Legendre polynomials

Extra keywords: (Gr-96:3.25)

12. The Gram-Schmidt procedure can be used to construct a set of orthonormal vectors by linear combination from a set of linearly independent, but non-orthonormal, vectors. It is a sort of brute force approach to use when more elegant methods of orthonormalization are not available.

The Gram-Schmidt procedure is as follows. Say $\{|\phi_n\rangle\}$ are a set of N linearly independent vectors that are **NOT** assumed to be orthonormal. One has ordered them in some reasonable manner indicated by the index n which increases from 1 to N. From this set we construct the orthonormal set $\{|\hat{u}_n\rangle\}$ of N normalized vectors where the hat symbol indicates their normalization. The unnormalized nth vector of the new set is given by

$$|u_n\rangle = |\phi_n\rangle - \sum_{\ell=1}^{n-1} |\hat{u}_\ell\rangle\langle\hat{u}_\ell|\phi_n\rangle \ ,$$

where the sum vanishes for $n=1$, and the corresponding normalized vector is given by

$$|\hat{u}_n\rangle = \frac{|u_n\rangle}{||u_n||} \ ,$$

where $||u_n|| = \sqrt{\langle u_n|u_n\rangle}$ is the norm of $|u_n\rangle$.

a) Prove the Gram-Schmidt procedure by induction.

b) In general there is an uncountable infinity of orthonormal sets that can be constructed from a non-orthonormal set. For example, consider ordinary vectors in 3-dimensional Euclidean space. By rotation of a orthonormal set of unit vectors an uncountable infinity of orthonormal sets of unit vectors can be created. Different orthonormal sets can be created using the Gram-Schmidt procedure just by itself. Say that there are N vectors in linearly independent non-orthonomcal set and each vector is orthogonal with all the others in the set. Show that you can create at least N different orthogonal sets by the Gram-Schmidt procedure.

c) Using the Gram-Schmidt procedure on the interval $[-1,1]$ (with weight function $w=1$ in the integral rule for the inner product) find the first three orthonormalized polynomial vectors starting from the linearly independent, but non-orthonomal set of polynomial vectors given by $\phi_n = x^n$ for integer $n \in [0,\infty)$. Show that the orthonormalized set are the first three normalized Legendre polynomials $\{\hat{P}_n(x)\}$. The normalized Legendre polynomials are given by

$$\hat{P}_n(x) = \sqrt{\frac{2n+1}{2}} P_n(x) \ ,$$

where $P_n(x)$ is a standard Legendre polynomial (e.g., Ar-547; WA-569). (Note an arbitrary phase factor $e^{i\theta}$ can also be multiplied to a normalized vector.) The reason why the Legendre polynomials arn't normalized is that the standard forms are what one gets straight from the generating function. The generating function approach to the Legendre polynomials allows you to prove many of their properties quickly (e.g., Ar-534, WA-553).

Table: Legendre Polynomials

Order n	P_n
0	$P_0 = 1$
1	$P_1 = x$
2	$P_2 = (1/2)(3x^2 - 1)$
3	$P_3 = (1/2)(5x^3 - 3x)$
4	$P_4 = (1/8)(35x^4 - 30x^2 + 3)$
5	$P_5 = (1/8)(63x^5 - 70x^3 + 15x)$

Note—The polynomials are from Ar-541 and WA-554. The degree of a Legendre polynomial is given by its order number n (WA-557).

d) The normalized Legendre polynomials form a complete orthonormal basis for piecewise continuous, normalizable functions in the interval $[-1, 1]$ (Ar-443). For a general polynomial of degree n, show that the expansion

$$Q_n(x) = \sum_{\ell=0}^{\infty} \hat{P}_\ell(x) \langle \hat{P}_\ell | Q_n \rangle$$

actually truncates at $\ell = n$. **HINT:** Consider x^n and how could construct it from Legendre polynomials starting with $P_n(x)$.

e) The part (c) result suggests that if the Gram-Schmidt procedure is continued beyond the first 3 vectors of the set $\{\phi_n\}$, one will continue getting the normalized Legendre polynomials in order. Prove this is so by comparing the Gram-Schmidt procedure result for $\langle \hat{P}_k | u_n \rangle$ and the expansion for $|u_n\rangle$ in the set $\{|\hat{P}_n\rangle\}$. In evaluating $\langle \hat{P}_k | u_n \rangle$, assume that the $|\hat{u}_\ell\rangle$ for $\ell < n$ are $|\hat{P}_\ell\rangle$. **HINT:** The part (d) result is also needed for the proof.

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007 qfull 00900 1 3 0 easy math: verifying a sinusoidal basis

Extra keywords: (Gr-96:3.26)

13. Consider the set of trigonometric functions defined by

$$f(x) = \sum_{n=0}^{N} [a_n \sin(nx) + b_n \cos(nx)]$$

on the interval $[-\pi, \pi]$. Show that the functions defined by

$$\phi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx} , \qquad \text{where} \qquad k = 0, \pm 1, \pm 2, \ldots, \pm N$$

are an orthonormal basis for the trigonometric set. What is the dimension of the space spanned by the basis?

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007 qfull 01000 2 3 0 moderate math: reduced SHO operator, Hermiticity

Extra keywords: (Gr-99:3.28), dimensionless simple harmonic oscillator Hamiltonian

14. Consider the operator

$$Q = -\frac{d^2}{dx^2} + x^2 \ .$$

   a) Show that $f(x) = e^{-x^2/2}$ is an eigenfunction of Q and determine its eigenvalue.

   b) Under what conditions, if any, is Q a Hermitian operator? **HINTS:** Recall

   $$\langle g|Q^\dagger|f\rangle^* = \langle f|Q|g\rangle$$

   is the defining relation for the Hermitian conjugate $Q^\dagger$ of operator Q. You will have to write the matrix element $\langle f|Q|g\rangle$ in the position representation and use integration by parts to find the conditions.

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007 qfull 01100 2 5 0 moderate thinking: Hilbert space problems

Extra keywords: (Gr-103:3.33)

15. Do the following.

   a) Show explicitly that any linear combination of two functions in the Hilbert space $L_2(a, b)$ is also in $L_2(a, b)$. (By explicitly, I mean don't just refer to the definition of a vector space which, of course requires the sum of any two vectors to be a vector.)

   b) For what values of real number s is $f(x) = |x|^s$ in $L_2(-a, a)$

   c) Show that $f(x) = e^{-|x|}$ is in $L_2 = L_2(-\infty, \infty)$. Find the wavenumber space representation of $f(x)$: recall the wavenumber "orthonormal" basis states in the position representation are

   $$\langle x|k\rangle = \frac{e^{ikx}}{\sqrt{2\pi}} \ .$$

---

007 qfull 01200 2 5 0 moderate thinking: Hermitian conjugate of AB

16. Some general operator and vector identities should be proven. Recall the definition of the Hermitian conjugate of general operator Q is giveny by

$$\langle\alpha|Q|\beta\rangle = \langle\beta|Q^\dagger|\alpha\rangle^* \ ,$$

where $|\alpha\rangle$ and $|\beta\rangle$ are general vectors.

   a) Prove that the bra corresponding to ket vector $Q|\beta\rangle$ is $\langle\beta|Q^\dagger$ for general Q and $|\beta\rangle$. **HINT:** Consider general vector $|\alpha\rangle$ and the inner product

   $$\langle\alpha|Q|\beta\rangle$$

   and work your way by valid steps to

   $$\langle\beta|Q^\dagger|\alpha\rangle^*$$

   and that completes the proof since

   $$\langle\alpha|\gamma\rangle = \langle\gamma|\alpha\rangle^*$$

   for general vectors $|\alpha\rangle$ and $|\gamma\rangle$.

   b) Show that the Hermitian conjugate of a scalar c is just its complex conjugate.

   c) Prove for operators, not matrices, that

   $$(AB)^\dagger = B^\dagger A^\dagger \ .$$

The result is, of course, consistent with matrix representations of these operators. But there are representations in which the operators are not matrices: e.g., the momentum operator in the position representation is differentiating operator

$$p = \frac{\hbar}{i}\frac{\partial}{\partial x} \ .$$

Our proof holds for such operators too since we've done the proof in the general operator-vector formalism.

d) Generalize the proof in part (c) for an operator product of any number.

e) Prove that $(A+B)^\dagger = A^\dagger + B^\dagger$.

f) Prove that $c[A,B]$ is a Hermitian operator for Hermitian A and B only when c is pure imaginary constant.

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007 qfull 01300 3 5 0 tough thinking: operators and matrices isomorphism

17. Expressions involving vector linear transformations or operators often (always?) isomorphic to the corresponding matrix expressions when the operators are represented by matrices in particular orthonormal bases. We would like to demonstrate this statement for a few important simple cases. For clarity express operators with hats (e.g., $\hat{A}$) and leave the corresponding matrices unadorned (e.g., A). Consider a general orthonormal basis $\{|i\rangle\}$ where i serves as a labeling index. Recall that the unit operator using this basis is

$$I = |i\rangle\langle i| \ ,$$

where we use the Einstein summation rule, and so there is a sum on i. Recall that the ijth matrix element of A is defined by

$$A_{ij} = \langle i|\hat{A}|j\rangle \ .$$

This definition means that the scalar product $\langle a|\hat{A}|b\rangle$, where $|a\rangle$ and $|b\rangle$ are general vectors, can be reexpressed by matrix expression:

$$\langle a|\hat{A}|b\rangle = \langle a|i\rangle\langle i|\hat{A}|j\rangle\langle j|b\rangle = a_i^* A_{ij} b_j = \vec{a}^\dagger A \vec{b} \ ,$$

where $\vec{a}$ and $\vec{b}$ are column vector n-tuples and where we have used the Einstein rule.

Prove that the following operator expressions are isomorphic to their corresponding matrix expressions.

a) Sum of operators $\hat{A}+\hat{B}$.

b) Product of operators $\hat{A}\hat{B}$.

c) Hermitian conjugation $\hat{A}^\dagger$.

d) The identity $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger$.

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007 qfull 01400 2 5 0 moderate thinking: bra ket projector completeness

Extra keywords: (Gr-118:3.57) See also CT-115, 138

18. For an inner product vector space there is some rule for calculating the inner product of two general vectors: an inner product being a complex scalar. If $|\alpha\rangle$ and $|\beta\rangle$ are general vectors, then their inner product is denoted by

$$\langle\alpha|\beta\rangle \ ,$$

where in general the order is significant. Obviously different rules can be imagined for a vector space which would lead to different values for the inner products. But the rule must have three basic properties:

$$(1) \qquad \langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^* \ ,$$

$$(2) \qquad \langle\alpha|\alpha\rangle \geq 0 \ , \qquad \text{where } \langle\alpha|\alpha\rangle = 0 \text{ if and only if } |\alpha\rangle = |0\rangle,$$

and

$$(3) \qquad \langle\alpha|\Big(b|\beta\rangle + c|\gamma\rangle\Big) = b\langle\alpha|\beta\rangle + c\langle\alpha|\gamma\rangle \ ,$$

where $|\alpha\rangle$, $|\beta\rangle$, and $|\gamma\rangle$ are general vectors of the vector space and b and c are general complex scalars.

There are some immediate corollaries of the properties. First, if $\langle\alpha|\beta\rangle$ is pure real, then

$$\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle \ .$$

Second, if $\langle\alpha|\beta\rangle$ is pure imaginary, then

$$\langle\beta|\alpha\rangle = -\langle\alpha|\beta\rangle \ .$$

Third, if

$$|\delta\rangle = b|\beta\rangle + c|\gamma\rangle \ ,$$

then

$$\langle\delta|\alpha\rangle^* = \langle\alpha|\delta\rangle = b\langle\alpha|\beta\rangle + c\langle\alpha|\gamma\rangle$$

which implies

$$\langle\delta|\alpha\rangle = b^*\langle\beta|\alpha\rangle + c^*\langle\gamma|\alpha\rangle \ .$$

This last result makes

$$\Big(\langle\beta|b^* + \langle\gamma|c^*\Big)|\alpha\rangle = b^*\langle\beta|\alpha\rangle + c^*\langle\gamma|\alpha\rangle$$

a meaningful expression. The 3rd rule for a vector product inner space and last corollary together mean that the distribution of inner product multiplication over addition happens in the normal way one is used to.

Dirac had the happy idea of defining dual space vectors with the notation $\langle\alpha|$ for the dual vector of $|\alpha\rangle$: $\langle\alpha|$ being called the bra vector or bra corresponding to $|\alpha\rangle$, the ket vector or ket: “bra” and “ket” coming from “bracket.” Mathematically, the bra $\langle\alpha|$ is a linear function of the vectors. It has the property of acting on a general vector $|\beta\rangle$ and yielding a complex scalar: the scalar being exactly the inner product $\langle\alpha|\beta\rangle$.

One immediate consequence of the bra definition can be drawn. Let $|\alpha\rangle$, $|\beta\rangle$, and a be general and let

$$|\alpha'\rangle = a|\alpha\rangle \ .$$

Then

$$\langle\alpha'|\beta\rangle = \langle\beta|\alpha'\rangle^* = a^*\langle\beta|\alpha\rangle^* = a^*\langle\alpha|\beta\rangle$$

implies that the bra corresponding to $|\alpha'\rangle$ is given by

$$\langle\alpha'| = a^*\langle\alpha| = \langle\alpha|a^* \ .$$

The use of bra vectors is perhaps unnecessary, but they do allow some operations and properties of inner product vector spaces to be written compactly and intelligibly. Let’s consider a few nice uses.

a) The projection operator or projector on to unit vector $|e\rangle$ is defined by

$$P_{\rm op} = |e\rangle\langle e| \ .$$

This operator has the property of changing a vector into a new vector that is $|e\rangle$ times a scalar. It is perfectly reasonable to call this new vector the component of the original vector in the direction of $|e\rangle$: this definition of component agrees with our 3-dimensional Euclidean definition of a vector component, and so is a sensible generalization of that the 3-dimensional Euclidean definition. This generalized component would also be the contribution of a basis of which $|e\rangle$ is a member to the expansion of the original vector: again the usage of the word component is entirely reasonable. In symbols

$$P_{\rm op}|\alpha\rangle = |e\rangle\langle e|\alpha\rangle = a|e\rangle \ ,$$

where $a = \langle e|\alpha\rangle$.

Show that $P_{\rm op}^2 = P_{\rm op}$, and then that $P_{\rm op}^n = P_{\rm op}$, where n is any integer greater than or equal to 1. **HINTS:** Write out the operators explicitly and remember $|e\rangle$ is a unit vector.

b) Say we have

$$P_{\rm op}|\alpha\rangle = a|\alpha\rangle \ ,$$

where $P_{\rm op} = |e\rangle\langle e|$ is the projection operator on unit vector $|e\rangle$ and $|\alpha\rangle$ is unknown non-null vector. Solve for the **TWO** solutions for a. Then solve for the $|\alpha\rangle$ vectors corresponding to these solutions. **HINTS:** Act on both sides of the equation with $\langle e|$ to find an equation for one a value. This equation won't yield the 2nd a value—and that's the hint for finding the 2nd a value. Substitute the a values back into the original equation to determine the corresponding $|\alpha\rangle$ vectors. Note one a value has a vast degeneracy in general: i.e., many vectors satisfy the original equation with that a value.

c) The Hermitian conjugate of an operator Q is written $Q^\dagger$. The definition of $Q^\dagger$ is given by the expression

$$\langle\beta|Q^\dagger|\alpha\rangle = \langle\alpha|Q|\beta\rangle^* \ ,$$

where $|\alpha\rangle$ and $|\beta\rangle$ are general vectors. Prove that the bra corresponding to ket $Q|\beta\rangle$ must $\langle\beta|Q^\dagger$ for general $|\alpha\rangle$. **HINTS:** Let $|\beta'\rangle = Q|\beta\rangle$ and substitute this for $Q|\beta\rangle$ in the defining equation of the Hermitian conjugate operator. Note operators are not matrices (although they can be represented as matrices in particular bases), and so you are not free to use purely matrix concepts: in particular the concepts of tranpose and complex conjugation of operators are not generally meaningful.

d) Say we define a particular operator Q by

$$Q = |\phi\rangle\langle\psi| \ ,$$

where $|\phi\rangle$ and $|\psi\rangle$ are general vectors. Solve for $Q^\dagger$. Under what condition is

$$Q^\dagger = Q \ ?$$

When an operator equals its Hermitian conjugate, the operator is called Hermitian just as in the case of matrices.

e) Say $\{|e_i\rangle\}$ is an orthonormal basis. Show that

$$|e_i\rangle\langle e_i| = \mathbf{1} \ ,$$

where we have used Einstein summation and $\mathbf{1}$ is the unit operator. **HINT:** Expand a general vector $|\alpha\rangle$ in the basis.

Chapt. 8 Operators, Hermitian Operators, Braket Formalism

Multiple-Choice Problems

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008 qmult 00090 1 4 5 easy deducto-memory: example Hilbert space

1. "Let's play *Jeopardy*! For \$100, the answer is: A space of all square-integrable functions on the x interval (a, b)."

   What is a ____________, Alex?

   a) non-inner product vector space   b) non-vector space   c) Dilbert space
   d) Dogbert space   e) Hilbert space

---

008 qmult 00100 1 1 3 easy memory: complex conjugate of scalar product

2. The scalar product $\langle f|g\rangle^*$ in general equals:

   a) $\langle f|g\rangle$.   b) $i\langle f|g\rangle$.   c) $\langle g|f\rangle$.   d) $\langle f|i|g\rangle$.   e) $\langle f|(-i)|g\rangle$.

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008 qmult 00200 1 4 3 easy deducto-memory: what operators do

3. "Let's play *Jeopardy*! For \$100, the answer is: It changes a vector into another vector."

   What is a/an ____________, Alex?

   a) wave function   b) scalar product   c) operator   d) bra
   e) telephone operator

---

008 qmult 00300 2 1 5 moderate memory: Hermitian conjugate of product

4. Given general operators A and B, $(AB)^\dagger$ equals:

   a) AB. b) $A^\dagger B^\dagger$.   c) A.   d) B.   e) $B^\dagger A^\dagger$.

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008 qmult 00400 2 5 5 moderate thinking: general Hermitian conjugation

5. The Hermitian conjugate of the operator $\lambda|\phi\rangle\langle\chi|\psi\rangle\langle\ell|A$ (with λ a scalar and A an operator) is:

   a) $\lambda|\phi\rangle\langle\chi|\psi\rangle\langle\ell|A$.   b) $\lambda|\phi\rangle\langle\chi|\psi\rangle\langle\ell|A^\dagger$.   c) $A|\ell\rangle\langle\psi|\chi\rangle\langle\phi|\lambda^*$.   d) $A|\ell\rangle\langle\psi|\chi\rangle\langle\phi|\lambda$.
   e) $A^\dagger|\ell\rangle\langle\psi|\chi\rangle\langle\phi|\lambda^*$.

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008 qmult 00500 1 1 5 easy memory: compatible observables

6. Compatible observables:

   a) anticommute.   b) are warm and cuddly with each other.   c) have no hair.
   d) have no complete simultaneous orthonormal basis.   e) commute.

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008 qmult 00600 1 1 3 easy memory: parity operator

7. The parity operator Π acting on $f(x)$ gives:

   df/dx.   b) $1/f(x)$.   c) $f(-x)$.   d) 0.   e) a spherical harmonic.

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008 qmult 00700 1 4 3 easy deducto-memory: braket expectation value

8. Given the position representation for an expectation value

$$\langle Q\rangle = \int_{-\infty}^{\infty} \Psi(x)^* Q \Psi(x)\, dx \ ,$$

what is the braket representation?

a) $\langle Q|\Psi^*|Q\rangle$. b) $\langle\Psi^*|Q|\Psi\rangle$. c) $\langle\Psi|Q|\Psi\rangle$. d) $\langle\Psi|Q^\dagger|\Psi\rangle$. e) $\langle Q|\Psi|Q\rangle$.

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008 qmult 00800 1 4 3 easy deducto-memory: Hermitian eigenproblem

9. What are the three main properties of the solutions to a Hermitian operator eigenproblem?

a) (i) The eigenvalues are pure **IMAGINARY**. (ii) The eigenvectors are guaranteed orthogonal, except for those governed by degenerate eigenvalues and these can always be orthogonalized. (iii) The eigenvectors **DO NOT** span all space.
b) (i) The eigenvalues are pure **REAL**. (ii) The eigenvectors are guaranteed orthogonal, except for those governed by degenerate eigenvalues and these can always be orthogonalized. (iii) The eigenvectors span all space in **ALL** cases.
c) (i) The eigenvalues are pure **REAL**. (ii) The eigenvectors are guaranteed orthogonal, except for those governed by degenerate eigenvalues and these can always be orthogonalized. (iii) The eigenvectors span all space for **ALL FINITE-DIMENSIONAL** spaces. In infinite dimensional cases they may or may not span all space. It is quantum mechanics postulate that the eigenvectors of an observable (which is a Hermitian operator) span all space.
d) (i) The eigenvalues are pure **IMAGINARY**. (ii) The eigenvectors are guaranteed orthogonal, except for those governed by degenerate eigenvalues and these can always be orthogonalized. (iii) The eigenvectors span all space in **ALL FINITE-DIMENSIONAL** spaces. In infinite dimensional cases they may or may not span all space.
e) (i) The eigenvalues are pure **REAL**. (ii) The eigenvectors are guaranteed orthogonal, except for those governed by degenerate eigenvalues and these can always be orthogonalized.

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008 qmult 00900 1 4 5 easy deducto-memory: definition observable

10. "Let's play *Jeopardy*! For \$100, the answer is: A physically significant Hermitian operator possessing a complete set of eigenvectors."

What is a/an ____________, Alex?

a) conjugate b) bra c) ket d) inobservable e) observable

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008 qmult 01000 1 4 4 easy deducto-memory: time-energy inequality

11. In the precisely-formulated time-energy inequality, the Δt is:

a) the standard deviation of time.
b) the standard deviation of energy.
c) a Hermitian operator.
d) the characteristic time for an observable's value to change by one standard deviation.
e) the characteristic time for the system to do nothing.

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008 qmult 02000 1 1 5 easy memory: common eigensets
Extra keywords: See CT-140ff

12. The statements "two observables commute" and "a common eigenset can be constructed for two observables" are

in flat contradiction. b) unrelated. c) in non-intersecting Venn diagrams. d) irrelevant in relation to each other. e) are equivalent in the sense that one implies the other.

Full-Answer Problems

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008 qfull 00010 1 1 0 easy memory: what is a ket?

1. What is a ket (representative general symbol $|\Psi\rangle$)?

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008 qfull 00015 1 1 0 easy memory: what is a bra?

2. What is a bra? (Representative general symbol $\langle\Psi|$.)

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008 qfull 00020 1 1 0 easy memory: why the braket formalism?

3. Why is quantum mechanics at the advanced level formulated in the braket formalism?

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008 qfull 00030 2 5 0 moderate thinking: Hermiticity and expectation values

Extra keywords: (Gr-94:3.21)

4. Recall the definition of Hermitian conjugate for a general operator Q is

$$\langle\alpha|Q|\beta\rangle = \langle\beta|Q^\dagger|\alpha\rangle^* \ ,$$

where $|\alpha\rangle$ and $|\beta\rangle$ are general vectors. If Q is Hermitian,

$$Q^\dagger = Q \ :$$

i.e., Q is its own Hermitian conjugate.

a) If Q is Hermitian, prove that the expectation value of a general vector $|\gamma\rangle$,

$$\langle\gamma|Q|\gamma\rangle \ ,$$

is pure real.

b) If the expectation value

$$\langle\gamma|Q|\gamma\rangle$$

is always pure real for general $|\gamma\rangle$, prove that Q is Hermitian. The statement to be proven is the converse of the statement in part (a). **HINT:** First show that

$$\langle\gamma|Q|\gamma\rangle = \langle\gamma|Q^\dagger|\gamma\rangle \ .$$

Then let $|\alpha\rangle$ and $|\beta\rangle$ be general vectors and construct a vector $|\xi\rangle = |\alpha\rangle + c|\beta\rangle$, where c is a general complex scalar. Note that the bra corresponding to $c|\beta\rangle$ is $c^*\langle\beta|$. Expand both sides of

$$\langle\xi|Q|\xi\rangle = \langle\xi|Q^\dagger|\xi\rangle \ ,$$

and then keep simplifying both sides making use of the first thing proven and the definition of a Hermitian conjugate. It may be useful to note that

$$(A^\dagger)^\dagger = A \qquad \text{and} \qquad (A+B)^\dagger = A^\dagger + B^\dagger \ ,$$

where A and B are general operators and You should be able to construct an expression where choosing $c = 1$ and then $c = i$ requires $Q = Q^\dagger$.

c) What simple statement follows from the proofs in parts (a) and (b)?

---

008 qfull 00032 2 5 0 moderate thinking: energy operator

5. We usually think of the Hamiltonian as being the "energy" operator, but term energy operator is also used for the operator

$$E_{\text{op}} = i\hbar\frac{\partial}{\partial t}$$

(Mo-184).

a) Find general expressions for the eigenvalues and normalizable eigenstates of E_{op}.

b) Show that E_{op} is not, in fact, a Hermitian operator in the space of physical wave functions. **HINT:** Recall the Hermitian conjugate of an operator Q is defined by

$$\langle\alpha|Q^\dagger|\beta\rangle = \langle\beta|Q|\alpha\rangle^*$$

(Gr-92), where $Q^\dagger$ is the Hermitian conjugate and $|\alpha\rangle$ and $|\beta\rangle$ are general vectors.

c) Is E_{op} formally a quantum mechanical observable? Does the projection postulate (Gr-105) on the measurement of energy apply to E_{op}? **HINT:** The last question is trickier than it seems.

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008 qfull 00040 2 3 0 moderate math: solving an eigenproblem

Extra keywords: (Gr-94:3.22) also diagonalizing a matrix.

6. Consider

$$Q = \begin{pmatrix} 1 & 1-i \\ 1+i & 0 \end{pmatrix} .$$

In this problem, we will diagonalize this matrix: i.e., solve for its eigenvalues and eigenvectors. We also actually explictly find the diagonal form—which is not usually necessary.

a) Is Q Hermitian?

b) Solve for the eigenvalues. Are they real?

c) Determine the normalized eigenvectors $\hat{a}$. Since eigenvectors are not unique to within a phase factor, the marker insists that you arrange your eigenvectors so that the first component of each is 1. Are the eigenvectors orthogonal? **HINT:** The matrix equation for the eigenvectors is a homogeneous matrix equation with non-trivial solutions (i.e., solutions that are not just zeros) for the eigenvalues since the determinant of $Q-\lambda I$ vanishes for those eigenvalues. However, 1 equation obtained from a $N \times N$ homogeneous matrix problem is always not independent: there are only $N-1$ independent equations and one can only solve for $N-1$ components of the eigenvectors. So if you set the first component of the solution vector to be 1, the $N-1$ equations allow you to solve for the other components. This solution vector is a valid solution vector, but its overall scale is arbitrary. There is no determined scale for the eigenvectors of a homogeneous matrix problem: e.g., k times solution vector $\vec{a}$ is also a solution. But, in quantum mechanics, physical vectors should be normalized and the normalization constraint provides an Nth independent equation, and thus allows a complete solution of the eigenvectors to within a global phase factor. Normalization doesn't set that global phase factor since it cancels out in the normalization equation. The global phase factor can be chosen arbitrarily for convenience. The global phase factor of a state no effect on the physics of the state.

d) Obtaining the eigenvalues and eigenvectors is usually all that is meant by diagonalization, but one can actually transform the eigenvalue matrix equation into a matrix equation where the matrix is diagonal and the eigenvectors can be solved for by inspection. One component of an eigenvector is 1 and the other components are zero. How does one transform to diagonal form? Consider our matrix equation

$$Q\hat{a} = \lambda\hat{a} .$$

Multipy both sides by the transformation matrix U to obtain

$$UQ\hat{a} = \lambda U\hat{a}$$

which is obviously the same as

$$UQU^{-1}U\hat{a} = \lambda U\hat{a} .$$

If we define

$$\hat{a}' = U\hat{a} \qquad \text{and} \qquad Q' = UQU^{-1} ,$$

then the transformed matrix equation is just

$$Q'\hat{a}' = \lambda\hat{a}' .$$

Prove that the transformation matrix U that gives the diagonalized matrix Q' just consists of rows that are the Hermitian conjugates of the eigenvectors. Then find the diagonalized matrix itself and its eigenvalue.

e) Compare the determinant $\det|Q|$, trace $\mathrm{Tr}(Q)$, and eigenvalues of Q to those of Q'.

f) The matrix U that we considered in part (d) is actually unitary. This means that

$$U^\dagger = U^{-1} .$$

Satisfy yourself that this is true. Unitary transformations have the useful property that inner products are invariant under them. If the inner product has a physical meaning and in particular the magnitude of vector has a physical meaning, unitary transformations can be physically relevant. In quantum mechanics, the inner product of a normalized state vector with itself 1 and this should be maintained by all physical transformations, and so such transformations must be unitary. Prove that

$$\langle a'|b'\rangle = \langle a|b\rangle$$

where

$$|a'\rangle = U|a\rangle|b'\rangle = U|b\rangle$$

and U is unitary.

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008 qfull 00500 2 5 0 moderate thinking: x-op in general formalism

Extra keywords: and k-op and p-op in general formalism too

7. The general formalism of quantum mechanics requires states to be vectors in Hilbert spaces and dynamical variables to be governed or determined (choose your verb) by observables (Hermitian operators with complete sets of eigenstates: i.e., sets that form a basis for the Hilbert space). These requirements are a Procrustian bed for the position, wavenumber (or momentum), and kinetic energy operators. These operators have complete sets of eigenvectors in a sense, but those eigenvectors arn't in any Hilbert space, because they can't be normalized. Nevertheless everything works out consistently if some identifications are made. The momentum and kinetic energy eigenstates are the same as the wavenumber eigenstates, and so we won't worry about them. The momentum and kinetic energy eigenvalues are different, of course.

NOTE: Procrustes (he who stretches) was a robber (or cannibal) with a remarkable bed that fit all guests—by racking or hacking according to whether small or tall. Theseus fit Procrustes to his own bed—and this was before that unfortunate incident with the Minotaur.

a) Consider the x_{op} eigenproblem in the general form

$$x_{\mathrm{op}}|x\rangle = x|x\rangle ,$$

where x is the eigenvalue and $|x\rangle$ is the eigenvector. The eigenvalues x and eigenvectors $|x\rangle$'s form continuous, not discrete, sets. The unity operator for the x_{op} basis is therefore

$$\mathbf{1} = \int dx\, |x\rangle\langle x| ,$$

where it is implied that the integral is over all space. An ideal measurement of position yields x and, by quantum mechanical postulate, puts the system is in state $|x\rangle$. But the system can't be really be in an unnormalizable state which is what the $|x\rangle$'s turn out to be. The system can be in an integral linear combination of such states.

Expand a general state $|\Psi\rangle$ in the $x_{\rm op}$ basis and identify what $|\Psi\rangle$ is in the position representation. Then identify what the inner product of two $x_{\rm op}$ eigenvectors $\langle x'|x\rangle$ must be. Why can't the $|x\rangle$ be in the Hilbert space? What is the position representation of $|x\rangle$? Prove that $x_{\rm op}$ in the position operator is just x itself.

b) Repeat part (a), *mutatis mutandis*, for $k_{\rm op}$.

c) What must $\langle x|k\rangle$ be? This is just an identification, not a proof—there are no proofs. **HINT:** Expand $|\Psi\rangle$ in the wavenumber representation and then operate on $|\Psi\rangle$ with $\langle x|$.

d) What is $\langle k|k'\rangle$ if we insert the position representation unit operator given the answer to part (c).

e) In order to have consistency with past work what must the matrix elements $\langle x|k_{\rm op}|x\rangle$, $\langle x|H_{\rm op}|x\rangle$, and $\langle k|x_{\rm op}|k\rangle$ be. Note these are just identifications, not proofs—there are no proofs. We omit $\langle k|H_{\rm op}|k\rangle$—you're not ready for $\langle k|H_{\rm op}|k\rangle$ as Jack Nicholson would snarl—if he were teaching intro quantum.

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008 qfull 00100 2 5 0 moderate thinking: expectation values two ways

Extra keywords: (Gr-108:3.35)

8. Consider the observable Q and the general **NORMALIZED** vector $|\Psi\rangle$. By quantum mechanics postulate, the expectation of Q^n, where $n \geq 0$ is some integer, for $|\Psi\rangle$ is

$$\langle Q^n\rangle = \langle\Psi|Q^n|\Psi\rangle \ .$$

a) Assume Q has a discrete spectrum of eigenvalues q_i and orthonormal eigenvectors $|q_i\rangle$. It follows from the general probabilistic interpretation postulate of quantum mechanics, that expectation value of Q^n for $|\Psi\rangle$ is given by

$$\langle Q^n\rangle = \sum_i q_i^n |\langle q_i|\Psi\rangle|^2 \ .$$

Show that this expression for $\langle Q^n\rangle$ also follows from the one in the preamble. What is $\sum_i |\langle q_i|\Psi\rangle|^2$ equal to?

b) Assume Q has a continuous spectrum of eigenvalues q and Dirac-orthonormal eigenvectors $|q\rangle$. (Dirac-orthonormal means that $\langle q'|q\rangle = \delta(q'-q)$, where $\delta(q'-q)$ is the Dirac delta function. The term Dirac-orthonormal is all my own invention: it needed to be.) It follows from the general probabilistic interpretation postulate of quantum mechanics, that expectation value of Q^n for $|\Psi\rangle$ is given by

$$\langle Q^n\rangle = \int dq\, q^n |\langle q|\Psi\rangle|^2 \ .$$

Show that this expression for $\langle Q^n\rangle$ also follows from the one in the preamble. What is $\int dq\, |\langle q|\Psi\rangle|^2$ equal to?

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008 qfull 00200 2 5 0 moderate thinking: simple commutator identities

9. Prove the following commutator identities.

a) $[A,B] = -[B,A]$.

b) $\left[\sum_i a_i A_i, \sum_j b_j B_j\right] = \sum_{ij} a_i b_j [A_i, B_j]$, where the a_i's and b_j's are just complex numbers.

c) $[A, BC] = [A, B]C + B[A, C]$.

d) $[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$. This has always seemed to me to be perfectly useless however true.

e) $(c[A, B])^\dagger = c^*[B^\dagger, A^\dagger]$, where c is a complex number.

f) The special case of the part (e) identity when A and B are Hermitian and c is pure imaginary. Is the operator in this special case Hermitian or anti-Hermitian?

---

008 qfull 00300 3 5 0 tough thinking: nontrivial commutator identities

Extra keywords: (Gr-111:3.41) but considerably extended.

10. Prove the following somewhat more difficult commutator identities.

a) Given

$$[B, [A, B]] = 0 \ , \qquad \text{prove} \qquad [A, F(B)] = [A, B]F'(B) \ ,$$

where A and B are general operators aside from the given condition and $F(B)$ is a general operator function of B. **HINTS:** Proof by induction is probably best. Recall that any function of an operator is (or is that should be) expandable in a power series of the operator: i.e.,

$$F(B) = \sum_{n=0}^{\infty} f_n B^n \ ,$$

where f_n are constants.

b) $[x, p] = i\hbar$.

c) $[x, p^n] = i\hbar n p^{n-1}$. **HINT:** Recall the part (a) answer.

d) $[p, x^n] = -i\hbar n x^{n-1}$. **HINT:** Recall the part (a) answer.

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008 qfull 01300 2 5 0 moderate thinking: general uncertainty principle

Extra keywords: Gr-108's proof

11. In quantum mechanics we believe that states are described by vectors in an abstract Hilbert space. The Hilbert space is an inner product vector space among other things.

An inner product vector space (as physicists view it anyway) has vectors written $|\alpha\rangle$ (the kets) and dual space vectors written $\langle\alpha|$ (the bras). We require that there is some rule such that the inner product operation

$$\langle\alpha|\beta\rangle$$

yields a complex number for general vectors $|\alpha\rangle$ and $|\beta\rangle$. The other properties required are:

$$\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^* \ ,$$

$$\langle\alpha|\alpha\rangle \geq 0 \ ,$$

where the equality holds if and only if $|\alpha\rangle = 0$ (i.e., $|\alpha\rangle$ is the null vector), and

$$\langle\alpha|(b|\beta\rangle + c|\gamma\rangle) = b\langle\alpha|\beta\rangle + c\langle\alpha\gamma\rangle \ .$$

The norm of a vector $|\alpha\rangle$ is defined by

$$||\alpha|| = \sqrt{\langle\alpha|\alpha\rangle} \ .$$

The vectors are transformed into new vectors by operators: e.g.,

$$|\alpha'\rangle = Q|\alpha\rangle \ ,$$

where Q is some operator. The Schwarz inequality

$$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$$

is a feature of inner product vector spaces. A concrete interpretation of the Schwarz inequality is that a vector must have a magnitude larger than or equal to any component of the vector along any axis. This can be seen by dividing the Schwarz inequality equality by

$$\langle\alpha|\alpha\rangle$$

assuming that $|\alpha\rangle$ is not null and interpreting

$$\langle\hat{\alpha}|\beta\rangle$$

as the component of $|\beta\rangle$ in the $|\hat{\alpha}\rangle$ direction where

$$|\hat{\alpha}\rangle = \frac{|\alpha\rangle}{||\alpha||} \ .$$

In quantum mechanics, the inner product operation in the 1-dimensional position representation, for example, is defined by

$$\langle\alpha|\beta\rangle = \int_{-\infty}^{\infty} \alpha(x)^*\beta(x)\,dx \ ,$$

where $\alpha(x)$ and $\beta(x)$ are square integrable functions. The dynamical variables of quantum mechanics are governed by physically relevant Hermitian operators with complete sets of eigenvectors. These operators, not too cogently, are called observables. The mean value or expectation value for an ensemble of identical states $|\alpha\rangle$ of a dynamical variable governed by an observable Q is given by

$$\langle\alpha|Q|\alpha\rangle \ .$$

The expectation value can be viewed as the overlap integral between the states $|\alpha\rangle$ and $Q|\alpha\rangle$.

The Hermitian conjugate $Q^\dagger$ of an operator Q is defined by

$$\langle\alpha|Q|\beta\rangle = \langle\beta|Q^\dagger|\alpha\rangle^* \ .$$

If $Q^\dagger = Q$, then Q is a Hermitian operator. Hermitian operators have only real expectation values. This follows from the general definition of Hermitian conjugation: if $Q^\dagger = Q$, then

$$\langle\alpha|Q|\alpha\rangle = \langle\alpha|Q|\alpha\rangle^* \ .$$

This result implies that the eigenvalues of a Hermitian operator are pure real since they are the expectation values of the eigenstates. We will not prove it here, but it is true also that non-degenerate eigenstates of a Hermitian operator are orthogonal and that the set of eigenstates of a Hermitian operator are a complete set guaranteed if the space is finite dimensional (Gr-93). But if the space is infinite dimensional completeness is not guaranteed for the set of eigenstates (Gr-99). The Hermitian operators with complete sets can be quantum mechanical observables.

Given the foregoing (and anything I've left out), the general uncertainty principle is a necessary consequence. This principle is

$$\sigma_A \sigma_B \geq \frac{1}{2}|\langle i[A,B]\rangle| \ ,$$

where A and B are observables, $[A,B] = AB - BA$ is the commutator of A and B, and σ_A and σ_B are standard deviations for observables A and B. The standard deviation squared (i.e., the variance) of A for a state $|\alpha\rangle$, for example, is given by

$$\sigma_A^2 = \langle\alpha|(A - \langle A\rangle)^2|\alpha\rangle \ ,$$

where $\langle A\rangle = \langle\alpha|A|\alpha\rangle$. Since A is a Hermitian operator, one can write

$$\begin{aligned}
\sigma_A^2 &= \langle\alpha|(A - \langle A\rangle)(A - \langle A\rangle)|\alpha\rangle \\
&= \langle\alpha|(A - \langle A\rangle)|f\rangle \\
&= \langle f|(A - \langle A\rangle)|\alpha\rangle \\
&= \langle f|f\rangle \ ,
\end{aligned}$$

where we have used the fact that expectation value of a Hermitian operator is real and have defined $|f\rangle = (A - \langle A\rangle)|\alpha\rangle$.

a) Define $|g\rangle = (B - \langle B\rangle)|\alpha\rangle$. Now prove that

$$\sigma_A^2\sigma_B^2 \geq |\langle f|g\rangle^2 \ .$$

b) Evaluate $\langle f|g\rangle$ in terms of expectation values of A and B for state $|\alpha\rangle$. For brevity the state can be left implied where convenient: i.e., $\langle A\rangle$ stands for $\langle\alpha|A|\alpha\rangle$, etc. Remember A and B are Hermitian and $\langle f|g\rangle$ is in general complex.

c) Show that for any complex number z

$$|z|^2 = [\mathrm{Re}(z)]^2 + [\mathrm{Im}(z)]^2 \ ,$$

where

$$\mathrm{Re}(z) = \frac{1}{2}(z + z^*) \qquad \text{and} \qquad \mathrm{Im}(z) = \frac{1}{2i}(z - z^*) \ .$$

Then evaluate

$$\mathrm{Re}(\langle f|g\rangle) \qquad \text{and} \qquad \mathrm{Im}(\langle f|g\rangle) \ .$$

d) In the classical analog case, A and B would just be dynamical variables whose statistical properties can be evaluated for some probability density. What does $\mathrm{Re}(\langle f|g\rangle)$ correspond to classically?

e) Now show that the general uncertainty inequality follows from the inequality you found in the part (a) answer. Is there a classical analog to the general uncertainty relation? Why or why not?

f) Given that A and B are Hermitian, show that $[A,B]$ is not Hermitian in general, but that $i[A,B]$ is.

g) Find the uncertainty relation for operators x and p: i.e., the Heisenberg uncertainty relation.

h) What relationship between states $|f\rangle$ and $|g\rangle$ will make the general uncertainty an equality?

i) Apply the relationship for equality to the case of x and p and obtain a differential equation for a one-dimensional state for which the Heisenberg uncertainty equality holds. Solve this differential equation for the minimum uncertainty wave packet. What kind of wave packet do you have? In what physical cases is the minimum uncertainty wave packet a solution to the Schrödinger equation.

j) Explain why the Heisenberg uncertainty equality is useful for understanding the ground states of many systems.

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008 qfull 01400 3 5 0 tough thinking: general uncertainty principle

Extra keywords: A dumb proof, and outdated by my current understanding.

12. You have a strange looking operator:

$$\ell = \frac{\delta Q}{\Delta Q} + i\frac{\delta R}{\Delta R} \ .$$

where Q and R are general Hermitian operators, ΔQ and ΔR are the standard deviations of Q and R, and

$$\delta Q \equiv Q - \langle Q \rangle \qquad \text{and} \qquad \delta R \equiv R - \langle R \rangle \ .$$

(a) Write down the Hermitian conjugate $\ell^\dagger$.

(b) Show $\ell^\dagger \ell$ a Hermitian operator and that it is a positive definite operator: i.e, that $\langle \ell^\dagger \ell \rangle \geq 0$. **HINT:** If you have to think about these results for more than a few seconds, then just assume them and go on.

(c) Multiply out $\ell^\dagger \ell$ and gather the cross terms into a commutator operator. Substitute for δQ and δR in the commutator using their definitions and simplify it.

(d) Evaluate the expectation value of the multiplied out $\ell^\dagger \ell$ operator. Simplify it remembering the definition of standard deviation.

(e) Remembering the positive definite result from part (b), find an inequality satisfied by $\Delta Q \Delta R$.

(f) Since the whole of the foregoing mysterious procedure could have been done with Q and R interchanged in the definition of ℓ, what second inequality must be satisfied by $\Delta Q \Delta R$.

(g) What third $\Delta Q \Delta R$ inequality is implied by two previous ones.

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008 qfull 01500 2 3 0 moderate math: x-H uncertainty relation

Extra keywords: (Gr-110:3.39)

13. Answer the following questions.

a) What is the uncertainty relation for operators x and H? Work it out until the expectation value is for the momentum operator p.

b) What is the time-dependent expression for any observable expectation value $\langle Q \rangle = \langle \Psi(t)|Q|\Psi(t) \rangle$ when the state $|\Psi(t)\rangle$ is expanded in the discrete set of stationary states (i.e., energy eigenstates) with their time-dependent factors included to allow for the time dependence of $|\Psi(t)\rangle$. Let the set of stationary states with explicit time dependence be $\{e^{-iE_j t/\hbar}|\phi_j\rangle\}$. Note functions of t commute with observables: observables may depend on time, but they don't contain time derivatives.

c) If state $|\Psi(t)\rangle$ from part (b) is itself the stationary state $e^{-iE_j t/\hbar}|\phi_j\rangle$, what the expectation value? Is the expectation value time independent?

d) Derive the special form of the uncertainty relation for operators x and H for the case of a stationary state of H? What, in fact, is σ_H for a stationary state? **HINT:** Remember Ehrenfest's theorem.

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008 qfull 01600 3 5 0 tough thinking: neutrino oscillation

Extra keywords: (Gr-120:3.58)

14. There are systems that exist apart from 3-dimensional Euclidean space: they are internal degrees of freedom such intrinsic spin of an electron or the proton-neutron identity of a nucleon (isospin: see, e.g., En-162 or Ga-429). Consider such an internal system for which we can only detect two states:

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{and} \qquad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \ .$$

This internal system is 2-dimensional in the abstract vector sense of dimensional: i.e., it can be described completely by an orthonormal basis of consisting of the 2 vectors we have just given. When we measure this system we force it into one or other of these states: i.e., we make the fundamental perturbation. But the system can exist in a general state of course:

$$|\Psi(t)\rangle = c_+(t)|+\rangle + c_-(t)|-\rangle = \begin{pmatrix} c_+(t) \\ c_-(t) \end{pmatrix} \ .$$

a) Given that $|\Psi(t)\rangle$ is **NORMALIZED**, what equation must the coefficients $c_+(t)$ and $c_-(t)$ satisfy.

b) For reasons only known to Mother Nature, the states we can measure (eigenvectors of whatever operator they may be) $|+\rangle$ and $|-\rangle$ are **NOT** eigenstates of the Hamiltonian that governs the time evolution of internal system. Let the Hamiltonian's eigenstates (i.e., the stationary states) be $|+'\rangle$ and $|-'\rangle$: i.e.,

$$H|+'\rangle = E_+|+'\rangle \qquad \text{and} \qquad H|-'\rangle = E_-|-'\rangle \ ,$$

where E_+ and E_- are the eigen-energies. Verify that the general state $|\Psi(t)\rangle$ expanded in these energy eigenstates,

$$|\Psi(t)\rangle = c_+e^{-iE_+t/\hbar}|+'\rangle + c_-e^{-iE_-t/\hbar}|-'\rangle$$

satisfies the general vector form of the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H|\Psi(t)\rangle \ .$$

HINT: This requires a one-line answer.

c) The Hamiltonian for this internal system has no differential operator form since there is no wave function. The matrix form in the $|+\rangle$ and $|-\rangle$ representation is

$$H = \begin{pmatrix} f & g \\ g & f \end{pmatrix} \ .$$

Given that H is Hermitian, prove that f and g must be real.

d) Solve for the eigenvalues (i.e., eigen-energies) of Hamiltonian H and for its normalized eigenvectors $|+'\rangle$ and $|-'\rangle$ in column vector form.

e) Given at $t = 0$ that

$$|\Psi(0)\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$$

show that

$$|\Psi(t)\rangle = \frac{1}{\sqrt{2}}(a+b)e^{-i(f+g)t/\hbar}|+'\rangle + \frac{1}{\sqrt{2}}(a-b)e^{-i(f-g)t/\hbar}|-'\rangle$$

and then show that

$$|\Psi(t)\rangle = e^{-ift/\hbar}\left[a\begin{pmatrix}\cos(gt/\hbar)\\ -i\sin(gt/\hbar)\end{pmatrix} + b\begin{pmatrix}-i\sin(gt/\hbar)\\ \cos(gt/\hbar)\end{pmatrix}\right] .$$

HINT: Recall the time-zero coefficients of expansion in basis $\{|\phi_i\rangle\}$ are given by $\langle\phi_i|\Psi(0)\rangle$.

f) For the state found given the part (e) question, what is the probability at any time t of measuring (i.e., forcing by the fundamental perturbation) the system into state

$$|+\rangle = \begin{pmatrix}1\\0\end{pmatrix} ?$$

HINT: Note a and b are in general complex.

g) Set $a = 1$ and $b = 0$ in the probability expression found in the part (f) answer. What is the probability of measuring the system in state $|+\rangle$? in state $|-\rangle$? What is the system doing between the two states?

NOTE: The weird kind of oscillation between detectable states we have discussed is a simple model of neutrino oscillation. Just as an example, the detectable states could be the electron neutrino and muon neutrino and the particle oscillates between them. Really there are three flavors of neutrinos and a three-way oscillation may occur. There is growing evidence that neutrino oscillation does happen. (This note may be somewhat outdated due to that growth of evidence.)

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008 qfull 01700 2 5 0 moderate thinking: operator product rule

Extra keywords: Reference Ba-134

15. A function of an operator A can be defined by a power series

$$f(A,\lambda) = \sum_{k=0}^{\infty} a_k(\lambda)A^k ,$$

where λ is an example of c-number parameter of the function and convergence is guaranteed by faith alone. For example, $e^{\lambda A}$ means that

$$e^{\lambda A} = \sum_{k=0}^{\infty} \frac{\lambda^k}{k!}A^k .$$

a) Show that a sensible definition of the derivative of $f(A,\lambda)$ with respect to λ is

$$\frac{df}{d\lambda} = \sum_{k=0}^{\infty} \frac{da_k}{d\lambda}A^k .$$

HINT: Differentiate a general matrix element of $f(A,\lambda)$.

b) Given the definition of the operator derivative of part (a), find product rule for operator derivatives. **HINT:** Differentiate a general matrix element of $f(A,\lambda)g(B,\lambda)$, where f and g are operator functions of general operators A and B.

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008 qfull 01800 3 5 0 hard thinking: common eigensets, CSCO

Extra keywords: See CT-139–144

16. One can always construct a common basis (or common eigenset) for commuting observables (i.e., Hermitian operators that allow complete eigensets). Let us investigate this property.

a) First, an easy problem. Say you are given obserables A and B and they have a common eigenset $\{|u^i_{a,b}\rangle\}$ such that

$$A|u^i_{a,b}\rangle = a|u^i_{a,b}\rangle \qquad \text{and} \qquad B|u^i_{a,b}\rangle = b|u^i_{a,b}\rangle ,$$

where a and b are eigenvalues and i labels different states that are degenerate with respect to both eigenvalues: i.e., have the same a and b eigenvalues. Thus specifying a, b, and i fully specifies a state. Show that A and B must commute.

b) Now you are given $[A, B] = 0$ and the eigenset of A $\{|u_a^i\rangle\}$, where i labels states that are degenerate with respect to eigenvalues a. Show that you can construct a common eigenset for A and B. **HINT:** Formally diagonalize B in the set $\{|u_a^i\rangle\}$ making use of commutation to show that many matrix elements are zero.

c) Say $\{A, B, C, \ldots\}$ constitutes a complete set of commuting operators (i.e., a CSCO). What can say about the common eigenset of $\{A, B, C, \ldots\}$?

Chapt. 9 Time Evolution and the Heisenberg Representation

Multiple-Choice Problems

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009 qmult 00100 1 4 1 moderate deducto-memory: constant of the motion

1. What are the conditions for observable Q to be a constant of the motion.

   a) $[H,Q]=0$ and $\partial Q/\partial t=0$.
   b) $[H,Q]\neq 0$ and $\partial Q/\partial t\neq 0$.
   c) $[H,Q]>0$ and $\partial Q/\partial t>0$.
   d) $[H,Q]<0$ and $\partial Q/\partial t<0$.
   e) $[H,Q]\geq 0$ and $\partial Q/\partial t\geq 0$.

Full-Answer Problems

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009 qfull 00100 3 5 0 tough thinking: time evolution, virial theorem

Extra keywords: (Gr-117:3.53, Gr2005-126:3.31) No one remembers Dorothy Lamour.

1. Answer the following questions that lead up to the proof of the virial theorem. **HINTS:** The answers to the earlier parts help answering the later parts. But you can still answer some later parts even if you don't get all the earlier parts.

   a) Given that $e^{-iE_n t/\hbar}|\phi_n\rangle$, a **STATIONARY STATE** (i.e., an eigen-energy state) of a time-independent Hamiltonian with its time-dependence factor explicitly shown, show that the expectation value for this state of any time-independent operator A is a constant with respect to time: i.e.,

   $$\frac{d\langle A\rangle}{dt}=0\ .$$

   HINT: This is easy.

   b) Given that $|\phi_n\rangle$ is a stationary state of H and A is a general operator (i.e., it doesn't have to be an observable or Hermitian), show that

   $$\langle\phi_n|[H,A]|\phi_n\rangle=0\ .$$

   HINT: This is not so hard. Recall the formal definition of the Hermitian conjugate of general operator A is

   $$\langle\alpha|A|\beta\rangle=\langle\beta|A^\dagger|\alpha\rangle^*\ .$$

   c) Prove that $[A,BC]=[A,B]C+B[A,C]$ for general operators A, B, and C.

   d) Prove $[x,p]=i\hbar$.

   e) Prove that

   $$[H,x]=-\frac{i\hbar}{m}p\ .$$

f) Prove that

$$[H,p] = i\hbar \left(\frac{\partial V}{\partial x}\right) .$$

g) Starting with the general time evolution equation (or general equation of motion) for general observable A

$$\frac{d\langle A\rangle}{dt} = \left\langle \frac{\partial A}{\partial t}\right\rangle + \frac{1}{\hbar}\langle i[H,A]\rangle$$

show that

$$\frac{d\langle xp\rangle}{dt} = 2\langle T\rangle - \left\langle x\frac{\partial V}{\partial x}\right\rangle ,$$

where $T = p^2/(2m)$ is the kinetic energy operator.

h) Show that

$$\frac{d\langle xp\rangle}{dt} = \frac{d\langle px\rangle}{dt} .$$

Whe quantity xp is the one-particle, one-dimensional virial operator. In classical physics, it would be a dynamical variable. **HINT:** This is easy.

i) Now for a **STATIONARY STATE** prove the 1-d virial theorem:

$$\langle T\rangle_{\text{stationary}} = \frac{1}{2}\left\langle x\frac{\partial V}{\partial x}\right\rangle_{\text{stationary}} .$$

HINT: Don't forget part (a) and what the general equation of motion says.

j) Given potential $V(x) \propto x^\lambda$, show that the virial theorem reduces to

$$\langle T\rangle_{\text{stationary}} = \frac{\lambda}{2}\langle V\rangle_{\text{stationary}} .$$

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009 qfull 01000 2 5 0 moderate thinking: Heis. Rep. evolution
Extra keywords: See Ba-137

2. Say A is an operator in the Schrödinger representation: this is the ordinary representation of beginning quantum mechanics. The Heisenberg representation of this operator for a system with Hamiltonian H is

$$A(t) = e^{iHt/\hbar}Ae^{-iHt/\hbar} ,$$

where $\exp(-iHt/\hbar)$ is operator function of H defined by

$$e^{-iHt/\hbar} = \sum_{\ell=0}^{\infty}\frac{1}{\ell!}\left(\frac{-iHt}{\hbar}\right)^{\ell} .$$

Show definitively that

$$\frac{dA(t)}{dt} = \frac{1}{i\hbar}[A(t),H] + \left(\frac{\partial A}{\partial t}\right)(t) ,$$

where the last term accounts for any implicit time dependence in A. **HINTS:** Take the time derivative of a general matrix element of $A(t)$ with the general states expanded in the eigenkets of H. Note that in the Heisenberg representation states don't have any time dependence: all the time-dependence is in the operators.

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009 qfull 01500 3 5 0 tough thinking: translation operator
Extra keywords: (Ba-145:2)

3. Here are some fun proofs to do that are all in the Schrödinger representation, except for the last one.

   a) Prove
   $$[\vec{r}, f(\vec{p}\cdot\vec{u})] = i\hbar\nabla_{\vec{p}} f(\vec{p}\cdot\vec{u}) \ ,$$
   where $\vec{u}$ is just a c-number vector (i.e., a vector consisting of ordinary scalar constant components) and the gradient operator is just a specially defined bit of formalism that means differentiate with respect to components of $\vec{p}$ to form a gradient as if they were ordinary variables. **HINT:** Recall
   $$f(\vec{p}\cdot\vec{u}) = \sum_{\ell=0}^{\infty} a_\ell (\vec{p}\cdot\vec{u})^\ell \ ,$$
   where the a_ℓ are some scalar coefficients and convergence is assumed.

   b) Using the part (a) result, prove that
   $$e^{i\vec{p}\cdot\vec{u}/\hbar}\vec{r}e^{-i\vec{p}\cdot\vec{u}/\hbar} = \vec{r} + \vec{u} \ .$$

   c) Now prove that
   $$|\Psi'\rangle = e^{-i\vec{p}\cdot\vec{u}/\hbar}|\Psi\rangle$$
   is the same state as $|\Psi\rangle$ translated by $\vec{u}$. In the position representation
   $$\Psi(\vec{r})' = e^{-i\vec{p}\cdot\vec{u}/\hbar}\Psi(\vec{r}) = \Psi(\vec{r} - \vec{u}) \ .$$

   d) Given
   $$|\Psi'\rangle = e^{-i\vec{p}\cdot\vec{u}/\hbar}|\Psi\rangle \ ,$$
   where $|\Psi'\rangle$ and $|\Psi\rangle$ are in the Heisenberg representation, show that $|\Psi'(t)\rangle$ (the state $|\Psi'\rangle$ in the Schrödinger representation) evolves according to
   $$|\Psi'(t)\rangle = e^{-i\vec{p}(-t)\cdot\vec{u}/\hbar}|\Psi(t)\rangle \ ,$$
   where $\vec{p}(-t)$ is the momentum operator in the Heisenberg representation at $-t$.

Chapt. 10 Measurement

Multiple-Choice Problems

010 qmult 00100 1 1 1 easy memory: fundamental perturbation

1. In an ideal quantum mechanical measurement of an observable A:

   a) the measurement always detects an **EIGENVALUE** of the observable and projects the system into an **EIGENSTATE** of the observable corresponding to that eigenvalue.
   b) the measurement always detects an **EXPECTATION VALUE** of the observable and projects the system into an **EIGENSTATE** of the observable.
   c) the measurement always detects an **EXPECTATION VALUE** of the observable and projects the system into an **NON-EIGENSTATE** of the observable.
   d) the measurement always detects an **3 EIGENVALUES** of the observable and projects the system into an **NON-EIGENSTATE** of the observable.
   e) The measurement always detects an **EXPECTATION VALUE** of the observable and projects the system into a **STATIONARY STATE**.

Full-Answer Problems

Multiple-Choice Problems

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011 qmult 00100 1 4 3 easy deducto-memory: central force

1. A central force is one which always points radially inward or outward from a fixed point which is the center of the central force. The magnitude of central force depends only on:

   a) the angle of the particle.
   b) the vector $\vec{r}$ from the center to the particle.
   c) the radial distance r from the center to the particle.
   d) the magnetic quantum number of the particle.
   e) the uncertainty principle.

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011 qmult 00200 1 1 2 easy memory: separation of variables

2. A usual approach to getting the eigenfunctions of a Hamiltonian in multi-dimensions is:

   a) non-separation of variables. b) separation of variables.
   c) separation of invariables. d) non-separation of invariables.
   e) non-separation of variables/invariables.

---

011 qmult 00210 1 1 3 easy memory: separation of variables 2

3. Say you have a differential equation of two independent variables x and y and you want to look for solutions that can be factorized thusly $f(x,y) = g(x)h(y)$. Say then it is possible to reorder equation into the form

$$\text{LHS}(x) = \text{RHS}(y) \ ,$$

   where LHS stands for left-hand side and RHS for right-hand side. Well LHS is explicitly independent of y and implicitly independent of x:

$$\frac{\partial \text{LHS}}{\partial y} = 0 \qquad \text{and} \qquad \frac{\partial \text{LHS}}{\partial x} = \frac{\partial \text{RHS}}{\partial x} = 0 \ .$$

   Thus, LHS is equal to a constant C and necessarily RHS is equal to the same constant C which is called the constant of separation (e.g., Arf-383). The solutions for $g(x)$ and $h(y)$ can be found separately and are related to each other through C. The solutions for $f(x,y)$ that cannot be factorized are not obtained, of course, by the described procedured. However, if one obtains complete sets of $g(x)$ and $h(y)$ solutions for the x-y region of interest, then any solution $f(x,y)$ can be constructed at least to within some approximation (Arf-443). Thus, the generalization of the described procedure is very general and powerful. It is called:

   a) separation of the left- and right-hand sides. b) partitioning.
   c) separation of the variables. d) solution factorization. e) the King Lear method.

---

011 qmult 00212 1 1 3 easy memory: separation of variables 3

4. Say you have a partial differential equation with independent variables x_i and you want to look for solutions that can be factorized thusly

$$f(\{x_i\}) = \prod f_i(x_i) \ .$$

   Now you substitute the factored form into the differential equation and find that it is possible to reorder differential equation into the form

$$g = \sum_j g_j(x_j) = \text{Constant} \ ,$$

where $g_j(x_j)$ is some formula depending on x_j only out of the set of variables $\{x_i\}$. The $g_j(x_j)$ function also depends in general on $f_j(x_j)$ and its derivatives. If we differentiate g with respect to general x_i, we find

$$\frac{\partial g}{\partial x_i} = \sum_j \frac{\partial g_j(x_j)}{\partial x_i} = \frac{\partial g_i(x_i)}{\partial x_i} = 0 \ ,$$

where we have used the fact that the variables are independent. Since x_i was general, we conclude that $g_i(x_i)$ is actually independent of x_i as well as all other independent variables. So all the $g_i(x_i)$ expressions, in fact, equal constants. These constants are called constants of separation. Thus, we have the set of ordinary differential equations

$$g_i(x_i) = C_i \ ,$$

where C_i is the constant of separation for variable i. The solutions for all $f_i(x_i)$ can now be looked for. The solutions $f(\{x_i\})$ that cannot be factorized are not obtained, of course, by the described procedured. However, if one obtains complete sets of solutions for each of the ordinary differential equations, then any solution $f(\{x_i\})$ can be constructed at least to within some approximation (Arf-443). Thus, the described procedure is very general and powerful. It is called:

a) separation of the g's. b) partitioning. c) separation of the variables.
d) the solution factorization. e) the King Lear method.

---

011 qmult 00300 1 4 2 easy deducto-memory: relative/cm reduction

5. "Let's play *Jeopardy*! For \$100, the answer is: By writing the two-body Schrödinger equation in relative/center-of-mass coordinates."

How do you ____________, Alex?

a) reduce a **ONE-BODY** problem to a **TWO-BODY** problem
b) reduce a **TWO-BODY** problem to a **ONE-BODY** problem
c) solve a one-dimensional infinite square well problem
d) solve for the simple harmonic oscillator eigenvalues
e) reduce a **TWO-BODY** problem to a **TWO-BODY** problem

---

011 qmult 00310 1 4 4 easy deducto-memory: reduced mass

6. The formula for the reduced mass m for two-body system (with bodies labeled 1 and 2) is:

a) $m = m_1 m_2$. b) $m = \dfrac{1}{m_1 m_2}$. c) $m = \dfrac{m_1 + m_2}{m_1 m_2}$. d) $m = \dfrac{m_1 m_2}{m_1 + m_2}$.
e) $m = \dfrac{1}{m_1}$.

---

011 qmult 00400 1 4 2 easy deducto memory: spherical harmonics 1

7. The eigensolutions of the angular part of the Hamiltonian for the central force problem are the:

a) linear harmonics. b) spherical harmonics. c) square harmonics.
d) Pythagorean harmonics. e) Galilean harmonics.

---

011 qmult 00410 1 4 4 easy deducto-memory: spherical harmonics 2
Extra keywords: mathematical physics

8. "Let's play *Jeopardy*! For \$100, the answer is: They form a basis or complete set for the 2-dimensional space of the surface a sphere which is usually described by the angular coordinates of spherical polar coordinates."

What are the ____________, Alex?

a) Hermite polynomials b) Laguerre polynomials
c) associated Laguerre polynomials d) spherical harmonics
e) Chebyshev polynomials

---

011 qmult 00420 1 4 3 easy deducto memory: spherical harmonic Y00

9. Just about the only spherical harmonic that people remember—and they really should remember it too—is Y_{00} =:

   a) $e^{im\phi}$. b) r^2. c) $\dfrac{1}{\sqrt{4\pi}}$. d) θ^2. e) $2a^{-3/2}e^{-r/a}$.

---

011 qmult 00500 1 4 2 easy deducto-memory: spdf designations

10. Conventionally, the spherical harmonic eigenstates for angular momentum quantum numbers

$$\ell = 0, 1, 2, 3, 4, \ldots$$

are designated by:

   a) *a*, *b*, *c*, *d*, *e*, etc.
   b) *s*, *p*, *d*, *f*, and then alphabetically following *f*: i.e., *g*, *h*, etc.
   c) *x*, *y*, *z*, *xx*, *yy*, *zz*, *xxx*, etc.
   d) A, C, B, D, E, etc.
   e) $@%&*!!

---

011 qmult 00510 1 4 3 easy deducto-memory: s electrons

11. "Let's play *Jeopardy*! For $100, the answer is: What the $\ell = 0$ electrons (or zero orbital angular momentum electrons) are called in spectroscopic notation."

   What are ____________, Alex?

   a) the Hermitian conjugates b) Herman's Hermits c) *s* electrons d) *p* electrons
   e) *h* electrons

Full-Answer Problems

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011 qfull 00100 2 5 0 moderate thinking: 2-body reduced to 1-body problem

Extra keywords: (Gr-178:5.1)

1. The 2-body time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m_1}\nabla_1^2\psi - \frac{\hbar^2}{2m_2}\nabla_2^2\psi + V_{\rm tot}\psi = E_{\rm total}\psi \ .$$

If the potential $V_{\rm tot} = V(\vec r\,) + V_{\rm cm}(\vec R\,)$ (where $\vec r = \vec r_2 - \vec r_1$ is the relative vector and $\vec R$ (the center of mass vector), then the problem can be separated into two problems: a relative problem 1-body equivalent problem and a center-of-mass 1-body equivalent problem. The center of mass vector is

$$\vec R = \frac{m_1\vec r_1 + m_2\vec r_2}{M} \ ,$$

where $M = m_1 + m_2$.

   a) Determine the expressions for $\vec r_1$ and $\vec r_2$ in terms of $\vec R$ and $\vec r$. Show how you do this.

   b) Determine the expressions for ∇_1^2 and ∇_2^2 in terms of $\nabla_{\rm cm}^2$ (the center-of-mass Laplacian operator) and ∇^2 (the relative Laplacian operator). Show how you do this. Then re-express the kinetic operator

$$-\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2$$

in terms of $\nabla^2_{\rm cm}$ and ∇^2. **HINTS:** The x, y, and z direction components of vectors can all be treated separately and identically since x components of $\vec{R}$ and $\vec{r}$) (i.e., X and x) depend only on x_1 and x_2, etc. You can introduce a reduced mass to make the transformed kinetic energy operator simpler.

c) Now separate the 2-body Schrödinger equation assuming $V_{\rm tot} = V(\vec{r}) + V_{\rm cm}(\vec{R})$. Show explicitly how the separation of variables is done. What are the solutions of the center-of-mass problem if $V_{\rm cm}(\vec{R}) = 0$? How would you interpret the solutions of the relative problem? **HINT:** I'm only looking for a short answer to the interpretation question.

---

011 qfull 00200 2 3 0 moderate math: central-force azimuthal component solution

Extra keywords: solving the azimuthal component of the central force problem

2. In the central force problem, the separated azimuthal part of the Schrödinger equation is:

$$\frac{d^2\Phi}{d\phi^2} = \kappa^2\Phi ,$$

where κ^2 is the constant of separation for the azimuthal part. The constant has been parameterized in terms of κ^2 because clairvoyance tells this is the good way.

a) Since the differential equation is second order, there should should be two independent solutions for each value of κ^2: i.e., the eigenvalue problem has degeneracy of 2 for the eigenvalue. Solve for the general solution Φ for each κ^2: i.e., the solution that is a linear combination of the two independent solutions with undetermined coefficients. Note that writing the separation constant as κ^2 is so far just a parameterization and nothing yet demands that κ^2 be greater than zero: it could be zero or less than zero. **HINT:** Use an exponential trial function. But do not forget the special case of $\kappa^2 = 0$.

b) Quantum mechanics that wave functions and their derivatives be continuous, except that discontinuities in derivatives are allowed when a potential goes to infinity which is just unreachable ideal limit. For our system, we are not allowing any infinite potentials. Our solutions and all order of derivatives are, in fact, continuous.

The space for azimuthal part is, in fact, finite, but unbounded. The coordinate $\phi = 0$ runs from 0 to 2π, but when you move 2π you are back where you started. So in a sense there are no boundary conditions. But quantum mechanics also demands that wave functions be single-valued. Since we have no interpretation for multi-valuedness, we micropostulate that it doesn't happen. The single-valuedness condition replaces the boundary conditions for the azimuthal part. Impose the single-valuedness condition on the general solution obtained in the part (a) answer and its derivative, and so that this leads to κ (not κ^2 note) must be an integer times the imaginary unit i. Remember to consider the special case where $\kappa^2 = 0$?

c) Writing im for κ where m is any integer, write down a general formula solution of the azimuthal part for a single m value. The solutions for m and $-|m|$ are the degenerate solutions for κ^2. By convention, no normalization constant is applied to the azimuthal part solutionsd: i.e., the coefficient of the special function that is the solution is left as just 1. The normalization is applied to the entire angular solutions which are the spherical harmonics. **HINT:** This is easy.

d) The orbital angular momentum z-component observable

$$L_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi} .$$

To be Hermitian this operator, the only allowed solutions must satisfy certain boundary conditions which for the interval $[0, 2\pi]$. The single-valuedness condition tells us these boundary conditions must be periodic boundary conditions. What are the eigen states for this observable that satisfy the periodic boundary conditions? Are the eigenvalues pure real as they should be? What is the relationship between these eigen states and thos of the azimuthal angle part we found in the part (c) answer?

e) Normalize the allowed eigensolutions of L_z Note these solutions are, in fact, conventionally left unnormalized: i.e., the coefficient of the special function that is the solution is left as just 1. Normalization is conventionally imposed on the total orbital angular momentum solutions, spherical harmonics.

011 qfull 01000 3 5 0 tough thinking: the nearly rigid rotator

3. You have a 3-dimensional system consisting of two distinct particles of masses m_1 and m_2. The two particles form a nearly rigid rotator. The relative time-independent Schrödinger equation for the system is:

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{L^2}{2\mu r^2}+V(r)\right]\Psi(r,\theta,\phi)=E\Psi(r,\theta,\phi) \ ,$$

where r, θ, and ϕ are the relative coordinates, $\mu = m_1 m_2/(m_1+m_2)$ is the reduced mass, and the potential is

$$V(r)=\begin{cases}0\ , & \text{for } r\in[a-\Delta a/2, a+\Delta a/2];\\ \infty\ , & \text{otherwise.}\end{cases}$$

a) Assume that Δa is so much smaller than a that $L^2/(2\mu r^2)\approx L^2/(2\mu a^2)$. Now separate the equation into radial and angular parts using E_{rad} and E_{rot} as the respective separation constants: $E_{\text{rad}}+E_{\text{rot}}=E$. Let the radial solutions be $R(r)$. You know what the angular solutions should be. Write down the separated equations.

b) For the radial equation assume that r varies so much more slowly than R over the region of non-infinite potential that

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)\approx\frac{\partial^2 R}{\partial r^2}$$

in that region. Change the coordinate variable to $x = r-(a-\Delta a/2)$ for simplicity: the non-infinite region of the potential then is then the x range $[0,\Delta a]$. With this approximation solve for the radial eigenstates and eigen-energies. Normalize the eigenstates. **HINTS:** Holy *déjà vue* all over again Batman, it's the 1-dimensional infinite square well problem. Don't mix up a and Δa.

c) Write down the eigenstates (just their general symbol, not expressions) and eigen-energy expression for the rotational equation. What is the degeneracy of each eigen-energy? **HINTS:** You shouldn't being trying to solve the equation. You should know what the eigenstates are.

d) Write the general expression for the total wave function. How many quantum numbers does it depend on?

e) Write down the general expression for the total energy. Which causes a greater change in energy: a change of 1 in the quantum number controling the radial energy or a change of 1 in the quantum number controling the rotational energy? Remember $\Delta a << a$ by assumption.

f) Sketch the energy level diagram.

Chapt. 12 The Hydrogenic Atom

Multiple-Choice Problems

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012 qmult 00050 1 1 1 easy memory: hydrogen atom, 2-body

1. The hydrogen atom is the simplest of all neutral atoms because:

   a) it is a 2-body system. b) it is a 3-body system. c) it has no electrons.
   d) it has many electrons. e) hydrogen is the most abundant element in the universe.

---

012 qmult 00100 1 1 3 easy memory: radial wave function requirements

2. What basic requirements must the radial part of hydrogenic atom wave function meet in order to be a physical radial wave function?

   a) Satisfy the radial part of the Schrödinger equation and grow exponentially as $r \to \infty$.
   b) Not satisfy the radial part of the Schrödinger equation and grow exponentially as $r \to \infty$.
   c) Satisfy the radial part of the Schrödinger equation and be normalizable.
   d) Not satisfy the radial part of the Schrödinger equation and be normalizable.
   e) None at all.

---

012 qmult 00190 1 1 2 easy memory: hydrogen wave functions

3. The hydrogenic atom eigenstate wave functions contain a factor that causes them to:

   a) increase exponentially with radius. b) decrease exponentially with radius.
   c) increase logarithmically with radius. d) increase quadratically with radius.
   e) increase linearly with wavelength.

---

012 qmult 00200 1 4 1 easy deducto-memory: associated Laguerre polyn.

4. What special functions are factors in the radial part of the of the hydrogenic atom eigenstate wave functions?

   a) The associated Laguerre polynomials. b) The unassociated Laguerre polynomials.
   c) The associated Jaguar polynomials. d) The unassociated jaguar polynomials.
   e) The Hermite polynomials.

---

012 qmult 01000 1 4 1 easy deducto-memory: atomic spectroscopy

5. Almost all would agree that the most important empirical means for learning about atomic energy eigenstates is:

   a) spectroscopy. b) microscopy. c) telescopy. d) pathology. e) astrology.

Full-Answer Problems

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012 qfull 00100 1 1 0 easy memory: separation of two body problem

1. The full Schrödinger equation for the hydrogenic atom is a function of two positions, one for the electron and one for the nucleus. What must one do to turn the problem into a central force problem for one body?

---

012 qfull 00200 2 5 0 moderate thinking: how does ¡r¿ vary with n?

2. How does the mean radius (expectation value radius) $\langle r\rangle_{n\ell m}$ for the hydrogenic atom vary with increasing n (i.e., with increasing energy)?

---

012 qfull 00300 2 1 0 moderate memory: H atom quantum numbers

3. What are the 3 quantum numbers of the hydrogenic atom derived from the spatial Schrödinger equation?

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012 qfull 00400 2 1 0 moderate memory: s electron polar plot

4. Sketch the polar plot for an s electron (i.e., an $\ell = 0$ electron)?

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012 qfull 00500 2 5 0 moderate thinking: rotating or standing wave functions

5. Are the hydrogenic wave functions Ψ_{nlm} rotating wave or standing wave functions?

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012 qfull 00600 2 5 0 moderate thinking: rotating or standing wave functions

6. Can there be hydrogenic atom stationary-state standing wave functions?

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012 qfull 00700 2 5 0 moderate thinking: what is the Bohr magneton?

7. What is the Bohr magneton?

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012 qfull 00800 2 5 0 moderate thinking: atomic magnetic moments

8. Why should an atom have a magnetic moment?

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012 qfull 00900 1 3 0 easy math: first 4 Laguerre polynomials keyword first 4 Laguerre polynomials, Rodrigues's formula

9. Using Rodrigues's formula for Laguerre polynomials (**NOT** Legendre polynomials) determine the first 4 Laguerre polynomials.

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012 qfull 01000 3 3 0 tough thinking : separation of external potential

Extra keywords: separation of external potential, 1st order expansion

10. Consider the initial hydrogenic-atom Schrödinger equation where the position variables are still for the nucleus and electron. Say we add perturbation potentials $V_{\rm n}(\vec r_{\rm n})$ for the nucleus and $V_e(\vec r_e)$ for the electron. We further specify that these perturbation potentials vary only linearly with position. How would one have to treat these potentials in order to transform to the center-of-mass/relative coordinate system and separate the Schrödinger equation? **HINTS:** Have you heard of the Taylor's series? You'll have to express the $\vec r_{\rm n}$ and $\vec r_e$ in terms of relative and center of mass coordinates.

---

012 qfull 01200 2 3 0 moderate math: s electron in nucleus

Extra keywords: (Gr-142:4.14)

11. Let us consider the probability that the electron of a hydrogenic atom in the ground state will be in the nucleus. Recall the wave function for ground state is

$$\Psi_{100}(\vec r) = R_{10}(r)Y_{00}(\theta,\phi) = 2a^{-3/2}e^{-r/a} \times \frac{1}{\sqrt{4\pi}}$$

(Gr2005-154), where $a = a_{\rm Bohr}[m_e/(mZ_{\rm N})]$: $a_{\rm Bohr} \approx 0.529$Å is the Bohr radius, $Z_{\rm N}$ is the nuclear charge, m_e is the electron mass, and m is the reduced mass of the actual hydrogenic atom.

a) First assume that the wave function is accurate down to $r = 0$. It actually can't be, of course. The wave function was derived assuming a point nucleus and the nucleus is, in fact, extended. However, the extension of the nucleus is of order 10^5 times smaller than the Bohr radius, and so the effect of a finite nucleus is a small perturbation. Given that the nuclear radius is b, calculate the probability of finding the electron in the nucleus. Use $\epsilon = b/(a/2) = 2b/a$ to simplify the formula. **HINT:** The formula

$$g(n,x) = \int_0^x e^{-t}t^n\,dt = n!\left(1 - e^{-x}\sum_{\ell=0}^{n}\frac{x^\ell}{\ell!}\right)$$

could be of use.

b) Expand the part (a) answer in ϵ power series and show to lowest non-zero order that

$$P(r < b, \epsilon << 1) = \frac{1}{6}\epsilon^3 = \frac{4}{3}\left(\frac{b}{a}\right)^3 \ .$$

c) An alternate approach to find the probability of the electron being in the nucleus is assume $\Psi(\vec{r})$ can be approximated by $\Psi(0)$ over nucleus. Thus

$$P(r < b) \approx \left(\frac{4\pi}{3}\right) b^3 |\Psi(0)|^2 \ .$$

Is this result consistent with the part (b) answer?

d) Assume $b \approx 10^{-15}$ m and $a = 0.5 \times 10^{-10}$ m. What is the approximate numerical value for finding the electron in the nucleus? You can't interpret this result as "the fraction of the time the electron spends in the nucleus". Nothing in quantum mechanics tells us that the electron spends time definitely anywhere. One should simply stop with what quantum mechanics gives: the result is the probability of finding the electron in nucleus.

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012 qfull 01300 3 5 0 tough thinking: derivation of quantum J current

Extra keywords: derivation of quantum $\vec{J}$ current, correspondence principle

12. Let's see if we can derive the probability current density from the correspondence principle. Note that the classical current density is given by $\vec{j}_{\rm cl} = \vec{v}_{\rm cl}\rho_{\rm cl}$. (a) First off we have to figure out what the quantum mechanical ρ and $\vec{j}$ are classified as in quantum mechanics? Are they operators or wave functions or expectation values or are they just their own things? Well they may indeed be just their own things, but one can interpret them as belonging to one of the three mentioned categories. Which? (b) Well now that part (a) is done we can use the correspondence principle to find an operator corresponding to classical $\vec{j}_{\rm cl}$. What are the the appropriate operators to replace the classical $\rho_{\rm cl}$ and $\vec{v}_{\rm cl}$ with (i.e., how are $\rho_{\rm cl}$ and $\vec{v}_{\rm cl}$ quantized)? (c) Have you remembered the quantization symmetrization rule? (d) Now go to it and derive the quantum mechanical $\vec{j}$. You might find the 3-d integration-by-parts rule handy:

$$\int_V \Psi\nabla\chi\,dV = \int_A \Psi\chi\,d\vec{A} - \int_V \nabla\Psi\chi\,dV \ ,$$

where $\int_V$ is for integral over all volume V and $\int_A$ is for integral over all vectorized surface area of volume V.

---

012 qfull 02100 1 3 0 easy math: positronium solution

13. Positronium is an exotic atom consisting of an electron and its antiparticle the positron. It was predicted to exist in 1934 (or even earlier) shortly after the positron was discovered in 1932. Positronium was experimentally discovered in 1951. Positronium cannot exist long because the electron and positron will mutually annihilate usually producing two γ-rays although more γ-rays are possible since there are multiple modes of annihilation. Positronium frequenctly forms in exited states and decays by radiative transitions to the ground state unless it annihilates first by some mode. Positronium transition spectra and annihilation γ-ray spectra provide a

fine test of quantum mechanics and quantum electrodynamics. Neglecting annihilation effects, spin effects, and relativistic effects, positronium to first order is Schrödinger-solution hydrogenic atom. We just consider this simplified positronium in this problem.

a) What are the positronium total mass and reduced mass?

b) What is the formula for the energy of the energy levels of positronium?

c) How does the emitted/absorbed photon of a positronium line transition (i.e., transition between energy levels) compare to the corresponding line transition photon of the Schrödinger-solution **HYDROGEN** atom? By "corresponding", we mean that the photons result from transitions that have the same initial and final principal quantum numbers.

Chapt. 13 General Theory of Angular Momentum

Multiple-Choice Problems

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013 qmult 00100 1 1 4 easy memory: ang. mom. commutation relations

1. The fundamental angular momentum commutation relation and a key corollary are, respectively:

   a) $[J_i, J_j] = 0$ and $[J^2, J_i] = J_i$. b) $[J_i, J_j] = J_k$ and $[J^2, J_i] = 0$.
   c) $[J_i, J_j] = 0$ and $[J^2, J_i] = 0$. d) $[J_i, J_j] = i\hbar\varepsilon_{ijk}J_k$ and $[J^2, J_i] = 0$.
   e) $[x_i, p_j] = i\hbar\delta_{ij}$, $[x_i, x_j] = 0$, and $[p_i, p_j] = 0$.

---

013 qmult 00910 1 1 3 easy memory: vector model

2. In the vector model for angular momentum of a quantum system with the standard axis for the eigenstates being the z axis, the particles in the eigenstates are thought of as having definite z-components of angular momentum $m_j\hbar$ and definite total angular momenta of magnitude $\sqrt{j(j+1)}\hbar$, where j can stand for orbital, spin, or total angular momentum quantum number and m_j is the z-component quantum number. Recall j can be only be integer or half-integer and there are $2j+1$ possible values of m_j given by $-j, -j+1, \ldots, j-1, j$. The x-y component of the angular momemementum has magnitude $\sqrt{j(j+1)-m_j^2}\hbar$, but it has no definite direction. Rather this component can be thought of as pointing all x-y directions in simultaneous: i.e., it is in a superposition state of all direction states. Diagramatically, the momentum vectors can be represented by

   a) cones with axis aligned with the x-axis. b) cones with axis aligned with the y-axis.
   c) cones with axis aligned with the z-axis.
   d) cones with axis aligned with the x-y-axis. e) the cones of silence.

---

013 qmult 01000 1 1 5 easy memory: rigid rotator eigen-energies

3. For a rigid rotator the rotational eigen-energies are proportional to:

   a) $\ell\hbar$. b) $\ell^2\hbar^2$. c) $\hbar^2/[\ell(\ell+1)]$. d) $\hbar^2/\ell^2$. e) $\ell(\ell+1)\hbar^2$.

---

013 qmult 02000 1 1 1 easy memory: added ang. mom. operators

4. Does the fundamental commutation relation for angular momentum operators (i.e., $[J_i, J_j] = i\hbar\varepsilon_{ijk}J_k$) apply to angular momentum operators formed by summation from angular momentum operators applying to individual particles or to spatial and spin degrees of freedom? The answer is:

   a) Yes. b) No. c) Maybe. d) All of the above. e) None of the above.

---

013 qmult 02100 1 4 5 easy deducto-memory: Clebsch-Gordan coefficients

5. "Let's play *Jeopardy*! For \$100, the answer is: The name for the coefficients used in the expansion of a total angular momentum state for 2 angular momentum degrees of freedom in terms of products of individual angular momemtum states."

   What are the ____________, Alex?

   a) Racah W coefficients b) Wigner $6j$ symbols c) Buck-Rogers coefficients
   d) Flash-Gordon coefficients e) Clebsch-Gordan coefficients

---

013 qmult 02200 1 4 5 easy deducto-memory: Clebsch-Gordan m rule

6. "Let's play *Jeopardy*! For \$100, the answer is: In constructing a set of $|j_1 j_2 jm\rangle$ states from a set of $|j_1 j_2 m_1 m_2\rangle$ states using Clebsch-Gordan coefficients, this is a strict constraint on the non-zero coefficients."

   What is the rule ____________, Alex?

   a) of complete overtures b) of incomplete overtures c) $m = m_1^2 + m_2^2$
   d) $m = m_1 - m_2$ e) $m = m_1 + m_2$

Full-Answer Problems

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013 qfull 00090 2 5 0 moderate math: kroneckar delta, Levi-Civita

1. There are two symbols that are very useful in dealing with quantum mechanical angular momentum and in many other contexts in physics: the Kronecker delta:

$$\delta_{ij} = \begin{cases} 1 \ , & i = j; \\ 0 \ , & i \neq j; \end{cases}$$

and the Levi-Civita symbol

$$\varepsilon_{ijk} = \begin{cases} 1 \ , & \text{if } ijk \text{ is a cyclic permutation of 123 (3 cases);} \\ -1 \ , & \text{if } ijk \text{ is an anticyclic permutation of 123 (3 cases);} \\ 0 \ , & \text{if any two indices are the same.} \end{cases}$$

NOTE: Leopold Kronecker (1823–1891) was a German mathematician although born in what is now Poland. Tullio Levi-Civita (1873–1941) was an Italian mathematician: the "C" in Civita is pronounced "ch".

a) Prove $\delta_{ij}\delta_{ik} = \delta_{jk}$, where we are using Einstein summation here and below, of course.

b) Now the toughie. Prove

$$\varepsilon_{ijk}\varepsilon_{i\ell m} = \delta_{j\ell}\delta_{km} - \delta_{jm}\delta_{k\ell} \ .$$

HINTS: I know of no simple one or two line proof. The best I've ever thought of was to consider cases where $jkm\ell$ span 3, 1, and 2 distinct values and to show that the two expressions are equal in all cases.

c) Now the cinchy one. Prove

$$\varepsilon_{ijk}\varepsilon_{ijm} = 2\delta_{km} \ .$$

d) What does $\varepsilon_{ijk}\varepsilon_{ijk}$ equal? Note there is Einstein summation on all indices now.

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013 qfull 00100 2 5 0 moderate thinking: angular momentum operator identities

2. Prove the following angular momentum operator identities. **HINT:** Recall the fundamental angular momentum commutator identity,

$$[J_i, J_j] = i\hbar\varepsilon_{ijk}J_k \ , \qquad \text{and the definition} \qquad J_\pm \equiv J_x \pm iJ_y \ .$$

a) $[J_i, J^2] = 0$.
b) $[J^2, J_\pm] = 0$.
c) $[J_z, J_\pm] = \pm\hbar J_\pm$.
d) $J_\pm^\dagger J_\pm = J_\mp J_\pm = J^2 - J_z(J_z \pm \hbar)$.

e)

$$J_x = \frac{1}{2}(J_+ + J_-) \qquad \text{and} \qquad J_y = \frac{1}{2i}(J_+ - J_-) \ .$$

f) $[J_+, J_-] = 2\hbar J_z$.

g)

$$J^2_{\left\{ {x \atop y} \right\}} = \pm\frac{1}{4}\left(J_+^2 + J_-^2 \pm \{J_+, J_-\}\right) \ ,$$

where the upper case is for J_x^2 and the lower case for J_y^2 and where recall that $\{A, B\} = AB + BA$ is the anticommutator of A and B.

h)

$$J^2 = \frac{1}{2}\{J_+, J_-\} + J_z^2 \ .$$

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013 qfull 00200 2 3 0 mod math: diagonalization of J_x for 3-d

Extra keywords: diagonalization of the J-x angular momentum matrix for 3-d

3. The x-component angular momentum operator matrix in a three-dimensional angular momentum space expressed in terms of the z-component orthonormal basis (i.e., the standard basis with eigenvectors $|1\rangle$, $|0\rangle$, and $|-1\rangle$) is:

$$J_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

(Co-659) and yes the $1/\sqrt{2}$ factor is correct. Is this matrix Hermitian? Diagonalize this matrix: i.e., solve for its eigenvalues and normalized eigenvectors (written in terms of the standard basis ket eigenvectors) or, if you prefer in column vector form. Note the solution is somewhat simpler if you solve the reduced eigen problem. Just divide both sides of the eigen equation by $\hbar/\sqrt{2}$ and solve for the reduced eigenvalues. The physical eigenvalues are the reduced ones times $\hbar/\sqrt{2}$. Verify that the eigenvectors are orthonormal.

NOTE: Albeit some consider it a sloppy notation since kets and bras are abstract vectors and columns vectors are from a concrete representation, its concretely useful to equate them at times. In the present case, the kets equate like so

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \ , \qquad |0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \ , \qquad |-1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \ ,$$

and the bras, like so

$$\langle 1| = (1,0,0)^* \ , \qquad \langle 0| = (0,1,0)^* \ , \qquad \langle -1| = (0,0,1)^* \ .$$

---

013 qfull 00300 2 3 0 mod math: diagonalization of J-y for 3-d

Extra keywords: diagonalization of the J-y angular momentum matrix for 3-d

4. The y-component angular momentum operator matrix in a three-dimensional angular momentum space expressed in terms of the z-component orthonormal basis (i.e., the standard basis with eigenvectors $|1\rangle$, $|0\rangle$, and $|-1\rangle$) is:

$$J_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

(Co-659) and yes the $1/\sqrt{2}$ factor is correct. Is this matrix Hermitian? Diagonalize this matrix: i.e., solve for its eigenvalues and normalized eigenvectors (written in terms of the standard basis kets) or, if you prefer in column vector form. Verify that the eigenvectors are orthonormal.

Note the solution is somewhat simpler if you solve the reduced eigen problem. Just divide both sides of the eigen equation by $\hbar/\sqrt{2}$ and solve for the reduced eigenvalues. The physical eigenvalues are the reduced ones times $\hbar/\sqrt{2}$.

NOTE: Albeit some consider it a sloppy notation since kets and bras are abstract vectors and columns vectors are from a concrete representation, its concretely useful to equate them at times. In the present case, the kets equate like so

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} , \qquad |0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} , \qquad |-1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} ,$$

and the bras, like so

$$\langle 1| = (1,0,0)^* , \qquad \langle 0| = (0,1,0)^* , \qquad \langle -1| = (0,0,1)^* .$$

---

013 qfull 00400 2 3 0 mod math: angular momemtum eqn. of motion

Extra keywords: (Gr-150:4.21) torque

5. Let's consider the angular momentum equation of motion in in the context of quantum mechanics.

   a) Prove that

   $$\frac{d\langle\vec{L}\,\rangle}{dt} = \langle\vec{\tau}\,\rangle ,$$

   where $\vec{L} = \vec{r} \times \vec{p}$ is the angular momentum operator and $\vec{\tau} = \vec{r} \times (-\nabla V)$ is the torque operator.

   b) Then prove that

   $$\frac{d\langle\vec{L}\,\rangle}{dt} = 0$$

   for any central potential system: i.e., a system where the potential depends on radius alone.

HINTS: You'll need to use the general time evolution equation—or equation of motion or derivative of expectation value: whatever one calls it—people do seem to avoid giving it a name. Then you will need to work out a commutation relation with a cross product operator. There are two approaches. First, show what the commutation relation is component by component. But that's for pedestrians. The second way is to use the Levi-Civita symbol with the Einstein summation rule to prove the all commutation relations simultaneously. Part (a) is most easily done using Cartesian coordinates and part (b) using spherical polar coordinates.

---

013 qfull 00500 2 3 0 moderate thinking: orbital angular momentum

Extra keywords: expectation values, standard deviations, quantum and classical analogs

6. Consider a spinless particle in an eigenstate $|\ell, m\rangle$ of the L^2 and L_z operators: ℓ is the L^2 quantum number and m the L_z quantum number. The set of $|\ell, m\rangle$ states are a complete orthonormal set for angular coordinates. Recall

$$\begin{aligned} L^2|\ell,m\rangle &= \ell(\ell+1)\hbar^2|\ell,m\rangle , \\ L_z|\ell,m\rangle &= m\hbar|\ell,m\rangle , \\ L_\pm|\ell,m\rangle &= \hbar\sqrt{\ell(\ell+1)-m(m\pm1)}|\ell,m\pm1\rangle , \end{aligned}$$

and

$$L_\pm = L_x \pm iL_y \ .$$

a) Solve for expectation values $\langle L_x \rangle$, and $\langle L_y \rangle$, and standard deviations ΔL_x and ΔL_y. **HINTS:** You will need expressions for L_x and L_y in terms of the given operators. Also the everything can be done by operator algebra: there is no need to bring in the spherical harmonics or particular representations of the operators.

b) Let us now see if there are classical analogs to the results in part (a). Let classical

$$L_z = m\hbar \ ,$$
$$L_x = \hbar\sqrt{\ell(\ell+1) - m^2}\cos(\phi)$$

and

$$L_y = \hbar\sqrt{\ell(\ell+1) - m^2}\sin(\phi) \ ,$$

where ϕ is the azimuthal angle of the angular momentum vector. Note $L_x^2 + L_y^2 + L_z^2 = \ell(\ell+1)$. Now solve for the classical $\langle L_x \rangle$ and $\langle L_y \rangle$, and the classical ΔL_x and ΔL_y assuming (i) that ϕ has a random uniform distribution the range $[0, 2\pi]$ and (ii) that $\phi = wt$ where ω is a constant angular frequency.

---

013 qfull 00600 2 5 0 moderate thinking: orb. ang. mon. commutator proofs

7. You are given the basic commutator identity $[r_i, p_j] = i\hbar\delta_{ij}$ and the correspondence principle result $\vec{L} = \vec{r} \times \vec{p}$.

a) Prove $[L_i, r_j] = i\hbar\varepsilon_{ijk}r_k$.

b) Prove $[L_i, p_j] = i\hbar\varepsilon_{ijk}p_k$.

c) Prove $[L_i, L_j] = i\hbar\varepsilon_{ijk}L_k$. **HINT:** Remember the old subtract and add the same thing trick.

d) Prove $[L_i, q_jq_j] = 0$, where $\vec{q}$ is any of $\vec{r}$, $\vec{p}$, and $\vec{L}$.

e) Prove $[L_i, Q_j] = i\hbar\varepsilon_{ijk}Q_k$ with $\vec{Q} = A\vec{q}B$, where A and B are any scalar combination of $\vec{r}$, $\vec{p}$, and $\vec{L}$: e.g., $A = r^{2k}p^{4m}L^{2n}\ldots$, where k, m, and n are integers.

f) Prove $[\hat{\alpha} \cdot \vec{L}, \vec{Q}] = i\hbar\vec{Q} \times \hat{\alpha}$, where $\hat{\alpha}$ is a constant c-number unit vector.

g) Show that

$$\frac{d\vec{Q}}{d\alpha} = \frac{i}{\hbar}[\hat{\alpha} \cdot \vec{L}, \vec{Q}]$$

is the differential equation for a right-hand-rule rotation by α of operator $\vec{Q}$ about the axis in the direction $\hat{\alpha}$. **HINT:** I'm not looking for mathematical rigor—but if you can do that it's OK.

h) Show that the solution of

$$\frac{d\vec{Q}}{d\alpha} = \frac{i}{\hbar}[\hat{\alpha} \cdot \vec{L}, \vec{Q}]$$

is

$$\vec{Q} = e^{i\vec{L}\cdot\vec{\alpha}/\hbar}\vec{Q}_0 e^{-i\vec{L}\cdot\vec{\alpha}/\hbar} \ ,$$

where $\vec{\alpha} = \alpha\hat{\alpha}$ is a general angle in vector form and $\vec{Q}_0$ is the inital operator $\vec{Q}$.

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013 qfull 02000 1 5 0 easy thinking: ang. mom. fundamental commutation

Extra keywords: for addition. Reference Ba-332.

8. The fundamental commutation relation of angular momentum can be generalized for multiple degrees of freedom. The degrees of freedom could be the angular momenta of multiple particles or the spatial and spin angular momenta of a particle or combinations thereof. Say we have degrees of freedom f and g, then the relation is

$$[J_{fi}, J_{gj}] = \delta_{fg} i\hbar\varepsilon_{ijk} J_{fk} \ .$$

We see that component operators refering to different degrees of freedom commute: this is true even in the case of indistinguishable particles. The total angular momentum operator $\vec{J}$ for a set of degrees of freedom with individual angular momentum operators $\vec{J}_f$ is, by the correspondence principle,

$$\vec{J} = \sum_f \vec{J}_f \ .$$

a) Prove that the fundamental commutation relation holds for the components of $\vec{J}$: i.e., prove

$$[J_i, J_j] = i\hbar\varepsilon_{ijk} J_k \ .$$

What does this result imply for summed angular momenta?

b) Now let $\vec{J} = \vec{J}_1 + \vec{J}_2$. Prove

$$J_\pm = J_{1\pm} + J_{2\pm} \ .$$

c) Prove

$$J^2 = J_1^2 + J_2^2 + J_{1+}J_{2-} + J_{1-}J_{2+} + 2J_{1z}J_{2z} \ .$$

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013 qfull 02100 3 5 0 hard thinking: Clebsch-Gordan ell plus 1/2

Extra keywords: See Ba-341 and CT-1020

9. One special case of great interest for which general formulae can be found for all Clebsch-Gordan coefficients is that of a general angular momentum added to a spin 1/2 angular momentum. Let the original angular momentum operators be labeled J_1^2, J_{1z}, J_2^2, and J_{2z}: the corresponding eigenvalues are $j_1(j_1+1)$, m_1, $(1/2)(1/2+1)$, and $\pm 1/2$. The set of product states of the original operators is $\{|j_1, 1/2, m_1, m_2 = \pm 1/2\rangle\}$. The summed operators are J^2 and J_z: the corresponding eigenvalues are j and m. The set of eigenstates of $\vec{J}_1^2$, J_2^2, J^2, and J_z is $\{|j_1, 1/2, j = j_1 \pm 1/2, m\rangle\}$. The expression for the Clebsch-Gordan coefficients is

$$\langle j_1, 1/2, m_1, m_2 = \pm 1/2 | j_1, 1/2, j = j_1 \pm 1/2, m\rangle \ .$$

a) For a given j_1 what are the possible j values?

b) Consider the trivial subspace for $j_1 = 0$. What are all the Clebsch-Gordan coefficients for this subspace.

c) Now consider the general subspace for $j_1 \geq 1/2$. First find the expression for the summed state with the largest m value. **HINT:** Recall

$$\langle j_1, j_2, m_1, m_2 | J_z | j_1, j_2, j, m\rangle = \langle j_1, j_2, m_1, m_2 | (J_{1z} + J_{2z}) | j_1, j_2, j, m\rangle \ ,$$

and so

$$m\langle j_1, j_2, m_1, m_2 | j_1, j_2, j, m\rangle = (m_1 + m_2)\langle j_1, j_2, m_1, m_2 | j_1, j_2, j, m\rangle \ .$$

Thus, the Clebsch-Gordan coefficient is zero unless $m = m_1 + m_2$.

d) Determine the expression for

$$|j_1, 1/2, j = j_1 + 1/2, m = j_1 - 1/2\rangle \ .$$

e) Now show that general expression for Clebsch-Gordan coefficient

$$\langle j_1, 1/2, m_1 = m - 1/2, m_2 = 1/2 | j_1, 1/2, j = j_1 + 1/2, m\rangle$$

is given by

$$\begin{aligned}&\langle j_1, 1/2, m_1 = m - 1/2, m_2 = 1/2 | j_1, 1/2, j = j_1 + 1/2, m\rangle \\ &= \sqrt{\frac{j_1(j_1+1) - (m+1/2)(m-1/2)}{(j_1+1/2)(j_1+3/2) - (m+1)m}} \sqrt{\frac{j_1(j_1+1) - (m+3/2)(m+1/2)}{(j_1+1/2)(j_1+3/2) - (m+2)(m+1)}} \cdots \\ &\qquad \sqrt{\frac{j_1(j_1+1) - j_1(j_1-1)}{(j_1+1/2)(j_1+3/2) - (j_1+1/2)(j_1-1/2)}} \ .\end{aligned}$$

HINT: What is mostly needed is a word argument.

f) Now show that

$$\begin{aligned}&\sqrt{\frac{j_1(j_1+1) - (m+1/2)(m-1/2)}{(j_1+1/2)(j_1+3/2) - (m+1)m}} \sqrt{\frac{j_1(j_1+1) - (m+3/2)(m+1/2)}{(j_1+1/2)(j_1+3/2) - (m+2)(m+1)}} \cdots \\ &\qquad \sqrt{\frac{j_1(j_1+1) - j_1(j_1-1)}{(j_1+1/2)(j_1+3/2) - (j_1+1/2)(j_1-1/2)}} \\ &= \sqrt{\frac{j_1 + m + 1/2}{2j_1 + 1}} \ .\end{aligned}$$

HINTS: Simplify

$$\sqrt{\frac{j_1(j_1+1) - (m+1/2)(m-1/2)}{(j_1+1/2)(j_1+3/2) - (m+1)m}}$$

by dividing top and bottom by a common factor. You might try $(Aj_1 + Bm + \ldots)(Cj_1 + Dm + \ldots)$ factorizations of the top and bottom.

g) Now show that the general expressions for the Clebsch-Gordan coefficients are

$$\langle j_1, 1/2, m_1 = m \mp 1/2, m_2 = \pm 1/2 | j_1, 1/2, j = j_1 + 1/2, m\rangle = \sqrt{\frac{j_1 \pm m + 1/2}{2j_1 + 1}}$$

$$\langle j_1, 1/2, m_1 = m \mp 1/2, m_2 = \pm 1/2 | j_1, 1/2, j = j_1 - 1/2, m\rangle = \mp \sqrt{\frac{j_1 \mp m + 1/2}{2j_1 + 1}} \ .$$

HINTS: Use the parts (e) and (f) answers and the normalization and orthogonality conditions.

h) The operator $\vec{J}_1 \cdot \vec{S}$ turns up in the spin-orbit interaction where $\vec{J}_1 = \vec{L}$. Show that the summed states $|j_1, 1/2, j = j_1 \pm 1/2, m\rangle$ are eigenstates of $\vec{J}_1 \cdot \vec{S}$. What are the eigenvalues?

Chapt. 14 Spin

Multiple-Choice Problems

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014 qmult 00100 1 4 5 easy deducto-memory: spin defined

Extra keywords: mathematical physics

1. "Let's play *Jeopardy*! For \$100, the answer is: It is the intrinsic angular momentum of a fundamental (or fundamental-for-most-purposes) particle. It is invariant and its quantum number s is always an integer or half-integer.

   What is ____________, Alex?

   a) rotation b) quantum number c) magnetic moment
   d) orbital angular momentum e) spin

---

014 qmult 00110 1 4 1 easy deducto-memory: Goudsmit and Uhlenbeck, spin

Extra keywords: Don't abbreviate: it ruins the joke

2. "Let's play *Jeopardy*! For \$100, the answer is: Goudsmit and Ulhenbeck."

   a) Who are the original proposers of electron spin in 1925, Alex?
   b) Who performed the Stern-Gerlach experiment, Alex?
   c) Who are Wolfgang Pauli's evil triplet brothers, Alex?
   d) What are two delightful Dutch cheeses, Alex?
   e) What were Rosencrantz and Gildenstern's first names, Alex?

---

014 qmult 00120 1 1 1 easy memory: spin magnitude

3. A spin s particle's angular momentum vector magnitude (in the vector model picture) is

   a) $\sqrt{s(s+1)}\hbar$. b) $s\hbar$ c) $\sqrt{s(s-1)}\hbar$ d) $-s\hbar$ e) $s(s+1)\hbar^2$

---

014 qmult 00130 1 1 5 easy memory: eigenvalues of spin 1/2 particle

4. The eigenvalues of a **COMPONENT** of the spin of a spin 1/2 particle are always:

   a) $\pm\hbar$. b) $\pm\dfrac{\hbar}{3}$. c) $\pm\dfrac{\hbar}{4}$. d) $\pm\dfrac{\hbar}{5}$. e) $\pm\dfrac{\hbar}{2}$.

---

014 qmult 00130 1 1 2 easy memory: eigenvalues of spin s particle

5. The quantum numbers for the component of the spin of a spin s particle are always:

   a) ± 1. b) $s, s-1, s-2, \ldots, -s+1, -s$. c) $\pm\dfrac{1}{2}$. d) ± 2. e) $\pm\dfrac{1}{4}$.

---

014 qmult 00140 1 4 2 easy deducto-memory: spin and environment

6. Is the spin (not spin component) of an electron dependent on the electron's environment?

   a) Always.
   b) No. Spin is an intrinsic, unchanging property of a particle.
   c) In atomic systems, no, but when free, yes.
   d) Both yes and no.
   e) It depends on a recount in Palm Beach.

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014 qmult 00400 1 4 5 easy deducto-memory: spin commutation relation

7. "Let's play *Jeopardy*! For \$100, the answer is:

$$[S_i, S_j] = i\hbar\varepsilon_{ijk}S_k \text{ .”}$$

What is ____________, Alex?

a) the spin anticommutator relation b) an implicit equation for ε_{ijk}
c) an impostulate d) an inobservable
e) the fundamental spin commutation relation

---

014 qmult 00500 1 4 2 easy deducto-memory: Pauli spin matrices

8. "Let's play *Jeopardy*! For \$100, the answer is:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \text{ .”}$$

What are ____________, Alex?

a) dimensioned spin 1/2 matrices b) the Pauli spin matrices
c) the Pauli principle matrices d) non-Hermitian matrices
e) matrix-look-alikes, not matrices

---

014 qmult 00600 1 1 1 easy memory: spin anticommutator relation

9. The expression

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}\mathbf{1}$$

is

a) the Pauli spin matrix anticommutator relation.
b) the Pauli spin matrix commutator relation.
c) the fundamental spin commutator relation.
d) the covariance of two standard deviations. e) an oddish relation.

---

014 qmult 00700 1 1 2 easy memory: spin rotation DE

10. The expression

$$\frac{d(\vec{S}\cdot\hat{n})}{d\alpha} = -\frac{i}{\hbar}[\vec{S}\cdot\hat{\alpha}, \vec{S}\cdot\hat{n}]$$

is a differential equation for

a) α.
b) the spin operator $\vec{S}\cdot\hat{n}$ as a function of rotation angle $\vec{\alpha}$.
c) $\hat{n}$.
d) the translation of the spin operator $\vec{S}$.
e) none of the above.

---

014 qmult 00800 1 4 5 easy deducto-memory: spin rotation operator

11. "Let's play *Jeopardy*! For \$100, the answer is:

$$U(\alpha) = e^{-i\vec{S}\cdot\vec{\alpha}/\hbar} = e^{-i\vec{\sigma}\cdot\vec{\alpha}/2} \text{ .”}$$

a) What the Hermitian conjugate of $U(-2\alpha)$, Alex?
b) What is a bra, Alex?
c) What is a spin 1/2 eigenstate, Alex?
d) What is the **NON-UNITARY** operator for the right-hand rule rotation of a spin 1/2 state by an angle α about the axis in the direction $\hat{\alpha}$, Alex?

e) What is the **UNITARY** operator for the right-hand rule rotation of a spin 1/2 state by an angle α about the axis in the direction $\hat{\alpha}$, Alex?

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014 qmult 00900 1 1 3 easy memory: space and spin operators commute

12. A spatial operator and a spin operator commute:

a) never. b) sometimes. c) always. d) always and never. e) to the office.

---

014 qmult 01000 2 1 4 moderate memory: joint spatial-spin rotation

13. The operator

$$U(\alpha) = e^{-i\vec{J}\cdot\vec{\alpha}/\hbar}$$

a) creates a spin 1/2 particle.
b) annihilates a spin 1/2 particle
c) left-hand-rule rotates both the space and spin parts of states by an angle α about an axis in the $\hat{\alpha}$ direction.
d) right-hand-rule rotates both the space and spin parts of states by an angle α about an axis in the $\hat{\alpha}$ direction.
e) turns a state into a U-turn state.

---

014 qmult 01100 1 4 5 easy deducto-memory: spin-magnetic interaction

14. "Let's play *Jeopardy*! For \$100, the answer is:

$$\vec{\mu} = g\frac{q}{2m}\vec{J}\ , \qquad \vec{F} = \nabla(\vec{\mu}\cdot\vec{B})\ , \qquad \vec{\tau} = \vec{\mu}\times\vec{B}\ , \qquad H = -\vec{\mu}\cdot\vec{B}\ ."$$

a) What are Maxwell's equations, Alex?
b) What are incorrect formulae, Alex?
c) What are classical formulae sans any quantum mechanical analogs, Alex?
d) What are quantum mechanical formulae sans any classical analogs, Alex?
e) What are formulae needed to treat the interaction of angular momentum of a particle and magnetic field in classical and quantum mechanics, Alex?

---

014 qmult 01200 1 1 2 easy memory: Bohr magneton

15. What is

$$\mu_{\rm B} = \frac{e\hbar}{2m_e} = 9.27400915(23)\times 10^{-24}\,{\rm J/T} = 5.7883817555(79)\times 10^{-5}\,{\rm eV/T}\ ?$$

a) The nuclear magneton, the characteristic magnetic moment of nuclear systems.
b) The Bohr magneton, the characteristic magnetic moment of electronic systems.
c) The intrinsic magnetic dipole moment of an electron.
d) The coefficient of sliding friction.
e) The zero-point energy of an electron.

---

014 qmult 01210 1 1 3 easy memory: g factor g-factor

16. The g factor in quantum mechanics is the dimensionless factor for some system that multiplied by the appropriate magneton (e.g., Bohr magneton for electron systems) times the angular momentum of the system divided by $\hbar$ gives the magnetic moment of the system. Sometimes the sign of the magnetic moment is included in the g factor and sometimes it is just shown explicitly. The modern way seems to be to include it, but yours truly finds that awkward and so for now yours truly doesn't do it. For the electron, the intrinsic magnetic moment operator associated with intrinsic spin is given by

$$\vec{\mu}_{\rm op} = -g\mu_{\rm B}\frac{\vec{S}_{\rm op}}{\hbar}\ ,$$

where μ_{B} is the Bohr magneton and S_{op} is the spin vector operator. What is g for the intrinsic magnetic moment operator of an electron to modern accuracy?

a) 1. b) 2. c) 2.0023193043622(15). d) 1/137. e) 137.

---

014 qmult 01210 1 1 4 easy memory: magnetic moment precession

Extra keywords: The precession is also called Larmor precession (En-114)

17. An object in a uniform magnetic field with magnetic moment due to the object's angular momentum will both classically and quantum mechanically:

a) Lancy progress. b) Lorenzo regress. c) London recess. d) Larmor precess.
e) Lamermoor transgress.

---

014 qmult 01300 1 1 3 easy memory: Zeeman effect

Extra keywords: See Ba-312 and Ba-466–468

18. What is an effect that lifts the angular momentum component energy degeneracy of atoms?

a) The spin-orbit effect.
b) The Paschen-Back effect or, for strong fields, the Zeman effect.
c) The Zeeman effect or, for strong fields, the Paschen-Back effect.
d) The Zimmermann effect.
e) The Zimmermann telegram.

---

014 qmult 01500 1 4 1 easy deducto-memory: spin resonance

Extra keywords: See Ba-317

19. "Let's play *Jeopardy*! For $100, the answer is: the effect in which a weak sinusoidal radio frequency magnetic field causes a particle with spin to precess about a direction perpendicular to strong uniform magnetic field that separates the spin component energy levels of the particle in energy."

a) What is spin magnetic resonance, Alex?
b) What is spin magnetic presence, Alex?
c) What is the preferred spin effect, Alex?
d) What is the dishonored spin effect, Alex?
e) What is the Zeeman effect, Alex?

---

014 qmult 01600 1 1 3 easy memory: spin resonance field

20. In spin magnetic resonance you can replace a rotating magnetic field by a sinusoidal one if you can neglect or filter:

a) magnetic fields altogether.
b) precession altogether.
c) the very **HIGH** frequency effects of the sinusoidal field.
d) spin altogether.
e) the very **LOW** frequency effects of the sinusoidal field.

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014 qmult 01700 1 4 5 easy deducto-memory: atomic clock

21. "Let's play *Jeopardy*! For $100, the answer is: The simplest of these consists of a beam of spinned particles that passes through two cavities each with crossed constant and sinusoidal magnetic fields."

What is a/an ____________, Alex?

a) Stern-Gerlach experiment b) Gentle-Gerlach experiment c) quartz-crystal
d) nuclear magnetic resonance machine e) atomic clock

---

014 qmult 01800 1 1 1 easy memory: second defined.

22. The spin state energy level separation of a ^{133}Ce atom used in an atomic clock to define the second corresponds by definition to a frequency of:

    a) 9 192 631 770 Hz.
    b) 3.141 592 65 Hz.
    c) 2.718 28 Hz.
    d) 0.577 215 66 Hz.
    e) 299 792 458 Hz.

Full-Answer Problems

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014 qfull 00100 2 5 0 moderate thinking: Pauli matrices in detail

1. The Pauli spin matrices are

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \qquad \text{and} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

a) Are the Pauli matrices Hermitian?

b) What is the result when Pauli matrices act on general vector

$$\begin{pmatrix} a \\ b \end{pmatrix} ?$$

c) Diagonalize the Pauli matrices: i.e., solve for their eigenvalues and **NORMALIZED** eigenvectors. **NOTE:** The verb 'diagonalize' takes its name from the fact that a matrix transformed to the representation of its own eigenvectors is diagonal with the eigenvalues being the diagonal elements. One often doesn't actually write the diagonal matrix explicitly.

d) Prove that

$$\sigma_i \sigma_j = \delta_{ij} \mathbf{1} + i\varepsilon_{ijk}\sigma_k ,$$

where i, j, and k stand for any of x, y, and z, $\mathbf{1}$ is the unit matrix (which can often be left as understood), δ_{ij} is the Kronecker delta, ε_{ijk} is the Levi-Civita symbol, and Einstein summation is used. **HINT:** I rather think by exhaustion is the only way: i.e., extreme tiredness.

e) Prove

$$[\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k \qquad \text{and} \qquad \{\sigma_i, \sigma_j\} = 2\delta_{ij} ,$$

where $\{\sigma_i, \sigma_j\} = \sigma_i\sigma_j + \sigma_j\sigma_i$ is the anticommutator of Pauli matrices. **HINT:** You should make use of the part (d) expression.

f) Show that a general 2×2 matrix can be expanded in the Pauli spin matrices plus the unit matrix: i.e.,

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \alpha \mathbf{1} + \vec{\beta} \cdot \vec{\sigma} ,$$

where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector of the Pauli matrices. **HINT:** Find expressions for the expansion coefficients α, β_x, β_y, and β_z.

g) Let $\vec{A}$ and $\vec{B}$ be vectors of operators in general and let the components of $\vec{B}$ commute with the Pauli matrices. Prove

$$(\vec{A} \cdot \vec{\sigma})(\vec{B} \cdot \vec{\sigma}) = \vec{A} \cdot \vec{B} + i(\vec{A} \times \vec{B}) \cdot \vec{\sigma} .$$

HINT: Make use of the part (d) expression.

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014 qfull 00110 1 3 0 easy math: diagonalization of y Pauli spin matrix

Extra keywords: (CT-203:2), but it corresponds to only part of that problem

2. The y-component Pauli matrix (just the y-spin matrix sans the $\hbar/2$ factor) expressed in terms of the z-component orthonormal basis (i.e., the standard z-basis with eigenvectors $|+\rangle$ and $|-\rangle$) is:

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} .$$

Diagonalize this matrix: i.e., solve for its eigenvalues and **NORMALIZED** eigenvectors written in terms of the standard z-basis eigenvector kets or, if your prefer, in column vector form for the z-basis. One doesn't have to literally do the basis transformation of the matrix to the diagonal form since, if one has the eigenvalues, one already knows what that form is. In quantum mechanics, literally doing the diagonalization of the matrix is often not intended by a diagonalization.

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014 qfull 00200 2 3 0 mod math: spin 1/2, spin $S_x + S_y$

Extra keywords: (Ga-241:9), spin 1/2, spin $S_x + S_y$, diagonalization

3. Consider a spin 1/2 system. Find the eigenvectors and eigenvalues for operator $S_x + S_y$. Say the system is in one of the eigen-states for this operator. What are the probabilities that an S_z measurement will give $\hbar/2$?

---

014 qfull 00250 2 5 0 moderate thinking: Euler formula for matrices

Extra keywords: Reference Ba-306, but I've generalized the result

4. Say that A is any matrix with the property that $A^2 = \mathbf{1}$, where $\mathbf{1}$ is the unit matrix. If we define e^{ixA} by

$$e^{ixA} = \sum_{\ell=0}^{\infty} \frac{(ixA)^\ell}{\ell!}$$

(where x is a scalar), show that

$$e^{ixA} = \mathbf{1}\cos(x) + iA\sin(x) .$$

This last expression is a generalization of Euler's formula (Ar-299).

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014 qfull 00300 3 5 0 tough thinking: rotation parameters

Extra keywords: (Ba-330:1b), but there is much more to this problem

5. The unitary spin 1/2 rotation operator is

$$U(\vec{\alpha}) = e^{-i\vec{S}\cdot\vec{\alpha}/\hbar} = e^{-i\vec{\sigma}\cdot\vec{\alpha}/2} ,$$

where $\vec{\alpha}$ is the vector rotation angle: $\vec{\alpha} = \alpha\hat{\alpha}$ with α being the angle of a right-hand rule rotation about the axis aligned by $\hat{\alpha}$. To rotate the spin component operator S_z from the z direction to the $\hat{n}$ direction one uses

$$\vec{S}\cdot\hat{n} = U(\vec{\alpha})S_zU(-\vec{\alpha})$$

(Ba-305) To rotate a z basis eigenstate into an $\hat{n}$ basis eigenstate one uses

$$|n\pm\rangle = U(\vec{\alpha})|z\pm\rangle$$

(Ba-306).

a) Expand $U(\vec{\alpha})$ into an explicit 2×2 matrix that can be used directly. Let the components of $\hat{\alpha}$ be written $\hat{\alpha}_x$, etc.

b) Now write out $U(\vec{\alpha})|z\pm\rangle$ explicitly.

c) You are given a general normalized spin vector

$$|\hat{n}+\rangle = \begin{pmatrix} a+ib \\ c+id \end{pmatrix} \ .$$

Find expressions for α and $\vec{\alpha}$ that yield this vector following a rotation of $|z+\rangle$. Then for those α and $\vec{\alpha}$ written in terms of a, b, c, and d, find the rotated $|z-\rangle$ state $|\hat{n}-\rangle$. Show explicitly that $|\hat{n}-\rangle$ is normalized and orthogonal to $|\hat{n}+\rangle$.

d) We gone so far: why quit now. Using our explicit matrix version of $U(\vec{\alpha})$ find explicit expressions for the components of $\hat{n}$ for a rotation from $\hat{z}$ in terms of α and the components of $\hat{\alpha}$. One has to solve for the components from

$$\vec{\sigma}\cdot\hat{n} = U(\vec{\alpha})\sigma_z U(-\vec{\alpha}) \ .$$

HINT: Write $U(\vec{\alpha})$ in simplified symbols until it's convenient to switch back to the proper variables: e.g.,

$$U(\vec{\alpha}) = \begin{pmatrix} a+ib & -c+id \\ c+id & a-ib \end{pmatrix} \ ,$$

where a, b, c, and d have the same meanings as you should have found in the part (c) answer.

---

014 qfull 00400 1 5 0 easy thinking: electron spin in B-field Hamiltonian

Extra keywords: electron spin in magnetic field Hamiltonian

6. What is the Hamiltonian fragment (piece, part) that describes the energy of an electron spin magnetic moment in a magnetic field? This fragment in a Schrödinger equation can sometimes be separated from the rest of the equation and solved as separate eigenvalue problem. Solve this separated problem. The intrinsic angular momentum operator is $\vec{S}$ and assume the magnetic field points in the z direction. **HINTS:** Think of the classical energy of a magnetic dipole in a magnetic field and use the correspondence principle. This is not a long question.

---

014 qfull 00500 2 5 0 moderate thinking: classical Larmor precession

7. Let's tackle the classical Larmor precession.

a) What is Newton's 2nd law in rotational form?

b) What is the torque on a magnetic dipole moment $\vec{\mu}$ in a magnetic field $\vec{B}$? **HINT:** Any first-year text will tell you.

c) Say that the magnetic moment of a system is given by $\vec{\mu} = \gamma\vec{L}$, where γ is the gyromagnetic ratio and $\vec{L}$ is the system's angular momemtum. Say also that there is a magnetic field $\vec{B} = (0, 0, B_z)$. Solve for the time evolution of $\vec{L}$ using Newton's 2nd law in rotational form assuming the **INITIAL CONDITION** $\vec{L}(t=0) = (L_{x,0}, 0, L_{z,0})$. **HINTS:** You should get coupled differential equations for two components of $\vec{L}$. They are not so hard to solve. For niceness you should define an appropriate Larmor frequency ω.

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014 qfull 00600 3 5 0 tough thinking: quantum mech. Larmor spin precession

Extra keywords: (Ba-330:1a), but there is much more to this problem

8. Consider a spin 1/2 particle with magnetic moment $\vec{M} = \gamma\vec{S}$. We put a uniform magnetic field in z direction: thus $\vec{B} = B_z\hat{z}$. As usual we take the z-basis as the standard basis for the problem.

a) Determine the normalized eigenstates for the S_x, S_y, and S_z operators in the z-basis. What are the eigenvalues?

b) Now expand the eigenvectors for S_z in the bases for S_x and S_y. You will need the expansions below.

c) If we consider only the spin degree of freedom, the Hamiltonian for the system is

$$H = -\vec{m}\cdot\vec{B} = -\gamma\vec{S}\cdot\vec{B} \ ,$$

where γ is a constant that could be negative or positive. Sometimes γ is called the gyromagnetic ratio (CT-389), but the expression gyromagnetic ratio is also used for the Landé g factor which itself has multiple related meanings. What are the eigenvalues and eigenvectors of H in the present case? **HINT:** Defining an appropriate Larmor frequency ω would be a boon further on.

d) The time-dependent Schrödinger equation in general is

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = H|\Psi\rangle \ .$$

What is the formal solution for $|\Psi(t)\rangle$ in terms of H and a given $|\Psi(0)\rangle$. **HINT:** Expand $|\Psi(0)\rangle$ in a the eigenstates of H which you are allowed to assume you know.

e) For our system you are given

$$|\Psi(0)\rangle = a_+|z+\rangle + a_-|z-\rangle \ .$$

What is $|\Psi(t)\rangle$? What are the probabilities for measuring spin up and down in the z direction and what is $\langle S_z\rangle$?

f) What are the probabilities for measuring spin up and down in the x direction and what is $\langle S_x\rangle$? Try to get nice looking expressions.

g) What are the probabilities for measuring spin up and down in the y direction and what is $\langle S_y\rangle$? Try to get nice looking expressions.

h) What can you say about the vector of spin expectation values given the answers to parts (f) and (g)?

i) Now given the initial state as $|x+\rangle$, what are $\langle S_x\rangle$, $\langle S_y\rangle$, and $\langle S_z\rangle$ in this special case?

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014 qfull 00700 2 5 0 tough thinking: spin algebra generalized

Extra keywords: (Ba-331:3)

9. Spin algebra can be used usefully for situations not involving spin. Say we have an atom or molecule with two isolated stationary states: i.e., there can be perturbation coupling and transitions between the two states, but no coupling to or transitions to or from anywhere else. Let the states be $|+\rangle$ and $|-\rangle$ with unperturbed energies ϵ_+ and ϵ_-; let $\epsilon_+ \geq \epsilon_-$. The states are orthonormal.

   a) Write the Hamiltonian for the states in matrix form and then decompose it into a linear combination of Pauli spin matrices and the unit matrix. What are the eigenstates $|+\rangle$ and $|-\rangle$ in column vector form? Note there is no spin necessarily in this problem: we are just using the Pauli matrices and all the tricks we have learned with them.

   b) Now we add a perturbation electric field in in the z direction: $E = E_0\cos(\omega t)$. You are given that the diagonal elements of the dipole moment matrix are zero and that the off diagonal elements are both equal to the real constant μ: i.e., $\mu = \langle +|ez|-\rangle = \langle -|ez|+\rangle$. Note μ can be positive or negative. Write down the Hamiltonian now.

   c) Write the Schrödinger equation for the perturbed system and then make a transformation that eliminates the unit matrix term from the problem. Do we ever really need to transform the state expressions back?

d) Show that a pretty explicit, approximate solution for the (transformed) Schrödinger equation is

$$|\Psi\rangle = e^{-i\omega t\sigma_z/2} e^{-i\Omega\hat{\sigma}t/2}|\Psi(0)\rangle \ ,$$

where

$$\Omega = \sqrt{(\omega_0-\omega)^2+\omega_1^2} \qquad \text{and} \qquad \hat{\sigma} = \frac{(\omega_0-\omega)}{\Omega}\sigma_z - \frac{\omega_1}{\Omega}\sigma_x \ .$$

The solution is valid near resonance: i.e., the case of $\omega \approx \omega_0$, where $\omega_0 \equiv (\epsilon_+ - \epsilon_-)/\hbar$. In order to get the solution we have averaged over times long enough to eliminate some of the high frequency behavior. To do this one assumes that $|\omega_1| = |\mu E_0/\hbar| << |\omega| \approx |\omega_0|$. **HINT:** The problem is pretty much isomorphic to the spin magnetic resonance problem.

e) Given that the initial state is $|+\rangle$, what are the probabilities that the system is in $|+\rangle$ and $|-\rangle$ at any later time? What are corresponding probabilities if the initial state is $|-\rangle$? Do any of these probabilities have high frequency behavior: i.e., time variation with frequency of order $\omega \approx \omega_0$ or greater?

f) The factor $e^{-i\omega t\sigma_z/2}$ in the solution

$$|\Psi\rangle = e^{-i\omega t\sigma_z/2} e^{-i\Omega\hat{\sigma}t/2}|\Psi(0)\rangle$$

is actually physically insufficient to give the high frequency behavior—although it is right in itself—since we dropped some high frequency behavior in deriving the solution. Thus any high frequency behavior predicted by the solution can't be physically accurate. You should have found in part (e) that the high frequency behavior from $e^{-i\omega t\sigma_z/2}$ canceled out of the probability expressions. Is there any reason for keeping the factor $e^{-i\omega t\sigma_z/2}$ in the formal solution? If there is a reason, what is it? **HINT:** There is a reason.

Chapt. 15 Time-Independent Approximation Methods

Multiple-Choice Problems

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015 qmult 00090 1 1 1 easy memory: quantum perturbation Santa

Extra keywords: the Christmas question

1. Santa Claus discovers that an intractable time-independent Schrödinger equation (i.e., a Hamiltonian eigen-problem) has an approximated form that is exactly solvable and has solutions that must be nearly those of the original problem. The approximated form eigen-solutions are also **NOT** degenerate. Not being a sage for nothing, Santa leaps to the conclusion that the original problem can now be solved by:

   a) non-degenerate time-independent perturbation theory.
   b) checking it twice.
   c) getting the elves to work on it.
   d) unthrottling the antlers,
   bidding Blixen to bound to the world's height,
   and chasing the dim stars,
   pass into nightness and out of all sight.
   e) peace on Earth and goodwill to humankind.

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015 qmult 00100 1 1 1 easy memory: time-independent perturbation

2. Non-degenerage time-independent perturbation theory assumes that the stationary states and eigen-energies of a time-independent system can be expanded in convergent power series in a perturbation parameter about, respectively:

   a) the stationary states and eigen-energies of another system called the unperturbed system.
   b) the eigen-energies and stationary states of a time-dependent system. c) the origin.
   d) the center. e) infinity.

---

015 qmult 00200 1 1 5 easy memory: zeroth order perturbation

3. The zeroth order perturbation of a system is:

   a) the most strongly perturbed system. b) the mostest strongly perturbed system.
   c) the deeply disturbed system. d) the negatively perturbed system
   e) the unperturbed system.

---

015 qmult 00300 1 1 2 easy memory: 1st order corrected energy

4. The formula

$$E_n^{\rm 1st} = E_n^{(0)} + \lambda\langle\psi_n^{(0)}|H^{(1)}|\psi_n^{(0)}\rangle$$

   in non-degenerate time-independent perturbation theory is the:

   a) 0th order corrected energy. b) 1st order corrected energy.
   c) 2nd order corrected energy. d) 1st order corrected state.
   e) 2nd order corrected state.

---

015 qmult 00400 1 4 4 easy deducto-memory: 1st order corrected state

5. The formula

$$|\psi_n^{\rm 1st}\rangle = |\psi_n^{(0)}\rangle + \lambda \sum_{\text{all } k, \text{ except } k\neq n} \frac{\langle\psi_k^{(0)}|H^{(1)}|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}} |\psi_k^{(0)}\rangle$$

in non-degenerate time-independent perturbation theory is the:

a) 0th order corrected energy. b) 1st order corrected energy.
c) 2nd order corrected energy. d) 1st order corrected state.
e) 2nd order corrected state.

---

015 qmult 00500 1 1 3 easy memory: 2nd order corrected energy

6. The formula

$$E_n^{\rm 2nd} = E_n^{(0)} + \lambda\langle\psi_n^{(0)}|H^{(1)}|\psi_n^{(0)}\rangle + \lambda^2 \sum_{\text{all } k, \text{ except } k\neq n} \frac{|\langle\psi_k^{(0)}|H^{(1)}|\psi_n^{(0)}\rangle|^2}{E_n^{(0)} - E_k^{(0)}}$$

in non-degenerate time-independent perturbation theory is the:

a) 0th order corrected energy. b) 1st order corrected energy.
c) 2nd order corrected energy. d) 1st order corrected state.
e) 2nd order corrected state.

---

015 qmult 00600 1 4 1 easy deducto-memory: degeneracy and perturbation

7. "Let's play *Jeopardy*! For \$100, the answer is: A common cause for the failure of time-independent perturbation theory—but failure can be recovered from with diagonalization."

What is ____________, Alex?

a) degeneracy b) tarnation c) subversion d) lunacy e) regency

---

015 qmult 01000 1 4 5 easy deducto-memory: diagonalization
Extra keywords: mathematical physics

8. "Let's play *Jeopardy*! For \$100, the answer is: A standard, non-perturbative approximate method of solving for the eigen-energies and stationary states of a system. If the system is in a finite Hilbert space, the method can be done for an exact solution."

What is ____________, Alex?

a) perturbation theory b) divagation c) strangulation d) triangulation
e) diagonalization

---

015 qmult 01020 1 1 2 easy memory: 2x2 eigenvalues

9. The values

$$E_\pm = \frac{1}{2}\left[(H_{11}+H_{22}) \pm \sqrt{(H_{11}-H_{22})^2 + 4|H_{12}|^2}\right]$$

are:

a) the stationary states of a 2 × 2 Hamiltonian matrix.
b) the eigen-energies of a 2 × 2 Hamiltonian matrix.
c) the eigen-energies of a 3 × 3 Hamiltonian matrix.
d) the stationary states of a 3 × 3 Hamiltonian matrix.
e) the 1st order non-degenerate perturbation correction energies.

Full-Answer Problems

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015 qfull 00080 2 5 0 moderate thinking: what is a perturbation?

1. What is a perturbation?

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015 qfull 0082 2 5 0 moderate thinking: basic perturbation hypothesis

2. What is the basic non-degenerate perturbation method hypothesis?

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015 qfull 00084 2 5 0 moderate thinking: smallness parameter

3. What is role of the smallness parameter in non-degenerate perturbation theory?

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015 qfull 00086 2 5 0 moderate thinking: 2nd bigger than 1st

4. If all the 2nd order non-degenerate perturbation corrections are greater than the 1st order ones, what might you suspect?

---

015 qfull 00088 2 5 0 moderate thinking: 2nd bigger than 1st all zero

5. If all the 2nd order non-degenerate perturbation corrections are greater than the 1st order ones, but the 1st order ones were all identically zero, what might you suspect?

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015 qfull 00190 2 5 0 tough thinking: 2nd order state correction

6. In non-degenerate time-independent perturbation theory, the 1st and 2nd order energy corrections for state i are, respectively,

$$E_i^{(1)} = \langle\psi_i^{(0)}|H^{(1)}|\psi_i^{(0)}\rangle \qquad \text{and} \qquad E_i^{(2)} = \sum_{\text{all } j, \text{ except } j\neq i} \frac{|\langle\psi_j^{(0)}|H^{(1)}|\psi_i^{(0)}\rangle|^2}{E_i^{(0)} - E_j^{(0)}}$$

and the 1st order state correction (which is not a state itself nor normalized in general) is

$$\begin{aligned}|\psi_i^{(1)}\rangle &= \sum_{\text{all } j, \text{ except } j\neq i} c_{ij}^{(1)}|\psi_j^{(0)}\rangle = \sum_{\text{all } j, \text{ except } j\neq i} \langle\psi_j^{(0)}|\psi_i^{(1)}\rangle|\psi_j^{(0)}\rangle \\ &= \sum_{\text{all } j, \text{ except } j\neq i} \frac{\langle\psi_j^{(0)}|H^{(1)}|\psi_i^{(0)}\rangle}{E_i^{(0)} - E_j^{(0)}}|\psi_j^{(0)}\rangle \ .\end{aligned}$$

The 2nd order corrected energy is

$$E_i^{\text{2nd}} = E_i^{(0)} + \lambda E_i^{(1)} + \lambda^2 E_i^{(2)}$$

and the 1st order corrected state is

$$|\psi_i^{\text{1st}}\rangle = |\psi_i^{(0)}\rangle + \lambda|\psi_i^{(1)}\rangle \ ,$$

where λ is the perturbation parameter. We have assumed that the set of states $\{|\psi_i^{(0)}\rangle\}$ is a complete orthonormal set of non-degenerate states.

But what is the 2nd order state correction? Let's see if we can find it.

a) The general equation for the nth order perturbation for a state i is

$$\sum_{k=n-1}^{n} H^{(n-k)}|\psi_i^{(k)}\rangle = \sum_{k=0}^{n} E_i^{(n-k)}|\psi_i^{(k)}\rangle \ .$$

Specialize this for the 2nd order (i.e., to $n = 2$) and expand the sums so that all the terms are shown explicitly.

b) Take the inner product of the part (a) answer with $|\psi_i^{(0)}\rangle$ and recover the formula for the 2nd order energy correction. Show the steps of the recovery. **HINT:** In order to get the answer, you will need to use a result for order $n = 1$ that follows from the normalization constraint on the full perturbation solution. The result is $\langle\psi_i^{(0)}|\psi_i^{(1)}\rangle = 0$.

c) The 2nd order state correction can be obtained from an expansion in the complete set of unperturbed states:

$$|\psi_i^{(2)}\rangle = \sum_k c_{ik}^{(2)}|\psi_k^{(0)}\rangle = \sum_k \langle\psi_k^{(0)}|\psi_i^{(2)}\rangle|\psi_k^{(0)}\rangle \ .$$

Now using the part (a) result, solve for

$$c_{ij}^{(2)} = \langle\psi_j^{(0)}|\psi_i^{(2)}\rangle$$

for the case of

$$j \neq i \ .$$

Write out the solution entirely in 0th order quantities, except for the perturbation Hamiltonian $H^{(1)}$.

d) The part (c) answer did not obtain the expansion coefficient

$$c_{ii}^{(2)} = \langle\psi_i^{(0)}|\psi_i^{(2)}\rangle \ .$$

To find this coefficient we need to make use a result for order $n = 2$ that follows from the normalization constraint on the full perturbation solution. For general $n \geq 1$, this constraint is

$$\sum_{m=0}^{n} \langle\psi_i^{(n-m)}|\psi_i^{(m)}\rangle = 0 \ ,$$

where

$$\langle\psi_i^{(0)}|\psi_i^{(k)}\rangle$$

is pure real for all k. Use the constraint for the case of $n = 2$ to find

$$c_{ii}^{(2)} = \langle\psi_i^{(0)}|\psi_i^{(2)}\rangle \ .$$

Write out the solution entirely in 0th order quantities, except for the perturbation Hamiltonian $H^{(1)}$. Simplify the result as much as reasonably possible.

---

015 qfull 01400 2 3 0 moderate math: infinite square well Dirac delta perturbation 1

Extra keywords: (Gr-225:6.1) Dirac delta perturbation, 1-dimensional infinite square well

7. Say you have a 1-dimensional infinite square well with

$$V(x) = \begin{cases} 0 & \text{for the } x \text{ range 0 to } a; \\ \infty & \text{otherwise.} \end{cases}$$

a) Solve for the eigen-states (i.e., stationary states) and eigen-energies from the time-independent Schrödinger equation. You must properly normalize the eigen-states states to answer part (b) correctly.

b) Say we add the Dirac delta function perturbation Hamiltonian

$$H^{(1)} = c\delta(x - a/2) \ .$$

What is the general expression for this perturbation for the first order perturbation energy correction for all eigen-states? Simplify the formula as much as possible.

---

015 qfull 01402 2 3 0 moderate math: infinite square well Dirac delta perturbation 2

Extra keywords: (Gr-225:6.1) Dirac delta perturbation, 1-dimensional infinite square well

8. Say you have a 1-dimensional infinite square well with

$$V(x)=\begin{cases}0 & \text{for the } x \text{ range 0 to } a;\\ \infty & \text{otherwise.}\end{cases}$$

The stationary states are

$$\psi_n(x)=\sqrt{\frac{2}{a}}\sin\left(k_n x\right) \ ,$$

where

$$k_n a = n\pi \qquad \text{and} \qquad k_n=\frac{n\pi}{a}$$

with $n=1,2,3,\ldots$ as allowed quantum numbers. The eigen-energies are

$$E_n=\frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 n^2 \ .$$

Say we add the Dirac delta function perturbation Hamiltonian

$$H^{(1)}=c\delta(x-a/2) \ .$$

What is the general formula for this perturbation for the first order perturbation energy correction for all eigen-states? Simplify the formula as much as possible.

---

015 qfull 01404 2 3 0 moderate math: infinite square well Dirac delta perturbation 3

Extra keywords: (Gr-225:6.1) Dirac delta perturbation, 1-dimensional infinite square well

9. Say you have a 1-dimensional infinite square well with

$$V(x)=\begin{cases}0 & \text{for the } x \text{ range 0 to } a;\\ \infty & \text{otherwise.}\end{cases}$$

The stationary states are

$$\psi_n(x)=\sqrt{\frac{2}{a}}\sin\left(k_n x\right) \ ,$$

where

$$k_n a = n\pi \qquad \text{and} \qquad k_n=\frac{n\pi}{a}$$

with $n=1,2,3,\ldots$ as allowed quantum numbers. The eigen-energies are

$$E_n^{\{0\}}=\frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 n^2 = E_1^{\{0\}} n^2 \ .$$

We now add the Dirac delta function perturbation Hamiltonian

$$H^{(1)}=c\delta(x-a/2) \ .$$

a) Can we use non-degenerate perturbation theory for the infinite square well? Why or why not?

b) What is the general formula for the perturbation for the 1st order perturbation energy correction for all eigen-states? Simplify the formula as much as possible.

c) Now evaluate a general matrix element for the perturbation

$$\langle\psi_m|H^{(1)}|\psi_n\rangle \ .$$

d) Simplify the general matrix element by inventing two simple functions of integer ℓ. The first is zero for ℓ even and 1 for ℓ odd. The second is 1 for k odd and -1 for k even where odd

$\ell = 2k + 1$ and k runs through all positive integers: i.e., $0, 1, 2, 3, \ldots$. **HINT:** If you this can't get this part, go on since the later parts don't require it.

e) Write out the 1st order perturbation correction formula for a general state n in as explicit and as simplified a form as reasonably possible. Note the correction is wanted, not the full 2nd order corrected state. **HINT:** Just leave the unperturbed states in the ket form $|\psi_n^0\rangle$. For compactness, one doesn't want to be explicit about them.

f) Write out the 2nd order perturbation correction formula for a general eigen-energy n in as explicit and as simplified a form as reasonably possible. Note the correction is wanted, not the full 2nd order corrected eigen-energy.

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015 qfull 01410 2 3 0 moderate math: 2-particle Dirac delta perturbation 1

10. You are give a complete set of orthonormal 1-dimensional single-particle states $\{\psi_n(x)\}$, where n is the indexing quantum number that determines energy. The state are **NOT** degenerate in energy. **NOTE:** Some parts of this problem can be done independently. So don't stop at any part that you can't immediately solve.

a) Now we need a general way to evaluate the eigen-energies for a symmetrized multi-particle state for a set of non-interacting identicle particles. The single-particle Hamiltonian H_i acting on single-particle state $\psi_n(x_i)$ gives

$$H_i \psi_n(x_i) = E_n \psi_n(x_i) \ .$$

A multi-particle state can be created from the single-particle states. Each particle for the multi-particle state has its own single-particle Hamiltonian H_i, but these Hamiltonians have identical formulae. For multi-particle state of I particles, the multi-particle Hamiltonian is

$$H_I = \sum_{i=1}^{I} H_i \ .$$

A product state (i.e., an unsymmetrized state) for I particles) is

$$\psi_{I,\mathrm{prod}} = \psi_{n_1}(x_1)\psi_{n_2}(x_2)\ldots\psi_{n_I}(x_I) \ .$$

This state though unphysical (since unsymmetrized) is an eigenstate of the multi-particle Hamiltonian. We find

$$H_I \psi_{I,\mathrm{prod}} = \left(\sum_{j=1}^{I} E_{n_j} \right) \psi_{I,\mathrm{prod}} \ ,$$

and so the eigen-energy of the product state is

$$E_I = \sum_{i=1}^{I} E_{n_i} \ ,$$

where the sum is over the set of n indexes that are in the product state.

What is the eigen-energy of the symmetrized state that is constructed from the product state? **HINT:** In symmetrizing the multi-particle state, the set of n_j indexes does not change. In the case of fermions, all n_j indexes are distinct. In the case of bosons, some n_j indexes may be the same: i.e., repeated single-particle states can occur in a product state. The answer is by inspection.

b) Say you have two non-interacting identical particles and a set of single-particle states for them. The particles could be bosons or fermions. If the particles are bosons, they are spinless. If the particles are fermions, they are in the same spin state. Thus, for both particles, we don't have to consider spin any further in this problem.

Give the general normalized symmetrized wave function for the two particles. Label the single-particle states m and n and the coordinates for the particles x_1 and x_2. Be sure the normalization is correct for both the $m \neq n$ and $m = n$ cases.

c) Now say we turn on a perturbation Hamiltonian

$$H^{(1)} = aV_0\delta(x_1 - x_2) \ ,$$

where a is a characteristic length, V_0 is strength factor, and $\delta(x_1 - x_2)$ is a Dirac delta function. The perturbation gives an interaction between the two particles. Determine the first order non-degenerate perturbation energy correction for the general two-particle state. Be as explicit as possible. **HINT:** For 2-dimensional space,

$$\langle\phi|Q|\psi\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi(x_1,x_2)^* Q\psi(x_1,x_2)\,dx_1\,dx_2 \ ,$$

where $|\phi\rangle$ and $|\psi\rangle$ are general states and Q is a general quantum mechanical observable (i.e., quantum mechanically relevant Hermitian operator).

d) Let's now specialize to the infinite square complete set of states. Recall the potential for the infinite square well is

$$V(x) = \begin{cases} 0 & \text{for the } x \text{ range 0 to } a; \\ \infty & \text{otherwise.} \end{cases}$$

The single-particle stationary states of this set are

$$\psi_\ell(x) = \sqrt{\frac{2}{a}}\sin\left(k_\ell x\right) \ ,$$

where

$$k_n a = \ell\pi \qquad \text{and} \qquad k_n = \frac{\ell\pi}{a}$$

with $\ell = 1, 2, 3, \ldots$ as allowed quantum numbers. The eigen-energies are

$$E_\ell = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 n^2 \ .$$

What is the energy for a general two-particle infinite-square-well state without perturbation? **HINT:** Remember the part (a) answer.

e) Determine the 1st order non-degenerate perturbation energy correction for the general two-particle infinite-square-well state. Be as explicit as possible. **HINT:** You will need a couple of trig identities:

$$\sin^2(A) = \frac{1}{2}[1 - \cos(2A)] \qquad \text{and} \qquad \cos(A)\cos(B) = \frac{1}{2}[\cos(A - B) + \cos(A + B)] \ .$$

Just keep going step by step carefully.

f) Using the part (e) answer, what are the 1st order non-degenerate perturbation energy corrections for the case of $m = n$ and the case of $m \neq n$.

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015 qfull 01412 3 5 0 tough thinking: 2-particle Dirac delta perturbation 2

Extra keywords: (Gr-226:6.3)

11. The single-particle stationary states and eigen-energies for a 1-dimensional infinite square well for region $[0,a]$ are, respectively,

$$\psi_n(x)=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)\qquad\text{and}\qquad E_n=\frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 n^2\ .$$

a) What is the expression for elementary 2-particle stationary states for **DISTINCT** spinless particles of the same mass? Label the particles 1 and 2 for convenience. Label the states n and n' for convenience too. What is the general expression for the energy of such 2-particle states? What are all the possible reduced energies $n^2+n'^2$ up to 100? These energies can be called energy levels: the levels may correspond to more than one state. What are are degeneracies of the energy levels? Remember the particles are **DISTINCT**. **HINT:** You are permitted to use a computer program to generate energy levels and degeneracies. But you can find them by hand too—a little tedious, but not hard if you go at it systematically.

b) Now suppose we turn on a perturbation potential for the non-identical particles of the form

$$H^{(1)}=V(x_1,x_2)=aV_0\delta(x_1-x_2)\ .$$

What is the expression for the diagonal matrix element

$$H_{(nn')(nn')}=\langle\psi_{nn'}(x_1,x_2)|H^{(1)}|\psi_{nn'}(x_1,x_2)\rangle\ ?$$

If you expand sine functions in exponentials evaluating, the matrix element is pretty easy, but you do have to treat the cases where $n\neq n'$ and $n=n'$ a bit differently.

Can you do perturbation theory on all the 2-particle states?

c) What is the expression for elementary 2-particle stationary states if we replace the distinct particles by identical spinless bosons? What is the general expression for the energy of such 2-particle states? (we have turned off the perturbation potential.) What are all the possible reduced energies $n^2+n'^2$ up to 100? These energies can be called energy levels: the levels may correspond to more than one state. What are are degeneracies of the energy levels? **HINT:** You don't have to do part (a) all over again, just *mutatis mutandis* it.)

d) Now suppose we turn on a perturbation potential of part (b) for the identical bosons. What is the expression for the diagonal matrix element

$$H_{(nn')(nn')}=\langle\psi_{nn'}(x_1,x_2)|H^{(1)}|\psi_{nn'}(x_1,x_2)\rangle\ ?$$

If you expand sine functions exponentials evaluating, the matrix element is pretty easy, but you do have to treat the cases where $n\neq n'$ and $n=n'$ a bit differently. Note the perturbation correction is a bit different from the distinct particle case. Why?

Can you do perturbation theory on all the 2-particle states?

e) What is the expression for elementary 2-particle stationary states if the 2 particles identical fermions with the same spin coordinate. Since the spin coordinates are identical, the spin part of the single-particle states are symmetrical. Don't bother writing down spinors or such. What is the general expression for the energy of such 2-particle states? What are all the possible reduced energies $n^2+n'^2$ up to 100? **HINT:** You don't have to do part (a) all over again, just *mutatis mutandis* it.)

f) Now suppose we turn on a perturbation potential of part (b) for the identical fermions. What is the expression for the diagonal matrix element

$$H_{(nn')(nn')}=\langle\psi_{nn'}(x_a,x_b)|H^{(1)}|\psi_{nn'}(x_a,x_b)\rangle\ .$$

Don't whine: this is easy if you see the trick. Why do you get the simple result you get? Can you do perturbation theory on all the 2-particle states?

g) What does the Dirac delta potential

$$V(x_a - x_b) = aV_0(x_a - x_b)$$

imply or do physically?

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015 qfull 01500 1 3 0 easy math: SHO 1st order perturbation cx

Extra keywords: SHO 1st order perturbation *cx*

12. Say you add a perturbation potential cx to a 1-dimensional simple harmonic oscillator (SHO) system. Calculate all the first order weak-coupling perturbation corrections for the eigen-energies. Recall the 1st order perturbation energy correction is given by

$$E_n^{(1)} = \langle\psi_n^{(0)}|H^{(1)}|\psi_n^{(0)}\rangle = 0 \ ,$$

where the $|\psi_n^0\rangle$ are unperturbed eigenstates. **HINT:** Think about the parity of SHO energy eigenstates.

---

015 qfull 01600 2 3 0 mod math: SHO exact cx perturbation

Extra keywords: (Gr-227:6.5), SHO, linear perturbation *cx*, exact cx solution

13. Say you added a perturbation $H^{(1)} = cx$ to the 1-dimensional simple harmonic oscillator (SHO) Hamiltonian, and so have

$$H = \frac{p^2}{2m} + \frac{1}{2}mw^2x^2 + cx$$

for the Hamiltonian. An exact solution to the time independent Schrödinger equation is, in fact, possible and easy since the new problem is still a SHO problem.

a) Let's consider just the mathematical aspects of the problem first. Given a quadratic

$$y = ax^2$$

with $a > 0$, where is its minimum and roots? Say you now add bx to get

$$y = ax^2 + bx \ .$$

Where are the minimum and roots now? By measuring the horizontal coordinate from a new origin it is possible to eliminate the linear dependence on the horizontal coordinate. Find this new origin. From a geometrical point of view what have you done by adding bx to $y = ax^2$: i.e., what has happened to the parabola on the plane? Sketch a plot of the original and translated parabolae and the curve $y = bx$. Why is should it be clear that adding the linear term bx that the mininum of the curve will be shifted downward?

b) Now that the math is clear what about the physics. What are the classical forces associated with the potentials

$$\frac{1}{2}m\omega^2x^2 \ , \qquad cx \ , \qquad \text{and} \qquad \frac{1}{2}m\omega^2x^2 + cx \ ?$$

What are the equilibrium points of the forces? What are the potential energies of the first and third equilibrium points? What has adding the cx potential done to the potential well of the SHO? How could you reduce the problem with the third potential to that with the first?

c) Now reduce time independent Schrödinger problem with the given Hamiltonian to the SHO problem. What are the solutions in terms of horizontal coordinate distance from the new origin and what are eigen-energies of the solutions? (I don't mean solve for the solutions. Just what are known solutions for reduced problem.)

015 qfull 01700 3 3 0 mod math: SHO and 2nd order perturbation cx

Extra keywords: SHO and 2nd order perturbation cx

14. Say you add a perturbation potential cx to a 1-dimensional simple harmonic oscillator (SHO) system. Give the formula for the 2nd order weak coupling perturbation correction for this special case simplified as much as possible. **HINT:** You will probably find the following matrix element formula for SHO eigenvectors useful:

$$\langle\Psi_k|x|\Psi_n\rangle = \begin{cases} \dfrac{1}{\beta}\sqrt{\dfrac{\max(k,n)}{2}} & \text{if } |k-n|=1; \\ 0 & \text{otherwise,} \end{cases}$$

where $\beta = \sqrt{m\omega/\hbar}$ (e.g., Mo-406).

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015 qfull 03000 3 3 0 tough math: SHO and 2nd order x^3 pre-perturbation

Extra keywords: SHO and 2nd order x^3 pre-perturbation

15. In preparation for calculating the 1st order perturbation wave function correction and the 2nd order perturbation energy correction for the 1-dimensional simple harmonic oscillator (SHO) system with perturbation potential cx^3, one needs to find a general expression for

$$\langle\psi_k|x^3|\psi_n\rangle \ .$$

Find this expression simplified as much as possible.

INSTRUCTIONS: You will need the following to formulae (which I hope are correct)

$$\frac{1}{\sqrt{2}\beta}\left[\sqrt{n+1}\psi_{n+1}(x) + \sqrt{n}\psi_{n-1}(x)\right] = x\psi_n(x)$$

and

$$\langle\psi_k|x^2|\psi_n\rangle = \begin{cases} \dfrac{2n+1}{2\beta^2} & \text{if } k=n; \\ \dfrac{\sqrt{[\max(k,n)-1]\max(k,n)}}{2\beta^2} & \text{if } |k-n|=2; \\ 0 & \text{otherwise,} \end{cases}$$

where $\beta = \sqrt{m\omega/\hbar}$. There are seven initial cases (one being zero) to find and five final cases after combining initial cases with same k and n relation. Write the expressions in terms of n, not k. You will simply have to work carefully and systematically to grind out the cases. What is the appropriate Kronecker delta function to go with each case so that one can put them in a sum over k in the 2nd order perturbation formulae? Make the Kronecker deltas in the form $\delta_{k,f(n)}$ where $f(n)$ is an expression like, e.g., $n-1$. Since k in the sum for the 2nd order perturbation runs only from zero to infinity is there any special treatment needed for including cases with Kronecker deltas like $\delta_{k,n-1}$ for $n=0$? **HINT:** Are such cases ever non-zero when they should be omitted?

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015 qfull 03100 3 3 0 mod math: SHO and 2nd order cx^3 perturbation

Extra keywords: SHO and 2nd order cx^3 perturbation

16. The following result is for simple harmonic oscillator eigenvectors:

$$\langle\psi_k|x^3|\psi_n\rangle = \frac{1}{2\sqrt{2}\beta^3}\begin{cases} 3(n+1)\sqrt{n+1} & \text{if } k=n+1 \text{ with } \delta_{k,n+1}; \\ 3n\sqrt{n} & \text{if } k=n-1 \text{ with } \delta_{k,n-1}; \\ \sqrt{(n+1)(n+2)(n+3)} & \text{if } k=n+3 \text{ with } \delta_{k,n+3}; \\ \sqrt{(n-2)(n-1)n} & \text{if } k=n-3 \text{ with } \delta_{k,n-3}; \\ 0 & \text{otherwise.} \end{cases}$$

Using this expression find the general expression for the SHO for the 2nd order weak-coupling perturbation corrections to the eigenstate energies for a perturbation potential cx^3. Why can you use the expression above without worrying about the fact that sum over states from zero to infinity doesn't include states with index less than zero.

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015 qfull 03110 2 5 0 moderate thinking: 4x4 eigenproblem/perturbation

17. You are given a zeroth order Hamiltonian matrix

$$H^{(0)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} .$$

a) Solve for the eigenvalues and normalized eigenvectors by inspection. You should label the states 1, 2, 3, and 4 for convenience. Is there any degeneracy and if so what are the degenerate states?

b) The evil wizard of physics now turns on a perturbation and the Hamiltonian becomes

$$H = \begin{pmatrix} 1 & \epsilon & 0 & 0 \\ \epsilon & 1 & 0 & 0 \\ 0 & 0 & 1 & \epsilon \\ 0 & 0 & \epsilon & -1 \end{pmatrix} ,$$

where ϵ is a small quantity. Solve for the exact eigenvalues and normalized eigenvectors in this case: i.e., diagonalize the perturbed Hamiltonian matrix. Is there any degeneracy now? **HINT:** Is there any reason why the two 2×2 blocks in the matrix cannot be treated as separate eigenvalue problems and the two-component eigenvectors extended trivially for the 4×4 problem?

c) Do non-degenerate perturbation theory to solve for the energy to 2nd order for those initial eigenstates which are **NOT** degenerate. **HINT:** All the perturbation matrix elements can be found in the part (b) **QUESTION**.

---

015 qfull 03300 3 5 0 tough thinking: perturbation and variation

Extra keywords: (Gr-235:6.9)

18. Consider quantum system of 3 dimensions with initial Hamiltonian

$$H^{(0)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

and perturbed Hamiltonian

$$H = \begin{pmatrix} 1-\epsilon & 0 & 0 \\ 0 & 1 & \epsilon \\ 0 & \epsilon & 2 \end{pmatrix} .$$

Note we assume $\epsilon << 1$. Also note that $H^{(0)}$ and H are matrix Hamiltonians: i.e., Hamiltonians in a particular representation. The matrix elements are $\langle\phi_i|H_{\rm op}^{(0)}|\phi_k\rangle$. $\langle\phi_i|H_{\rm op}|\phi_k\rangle$, respectively, where $H_{\rm op}^{(0)}$ and $H_{\rm op}$ are operator versions of the Hamiltonian and the set $\{|\phi_i\rangle\}$ is an orthonormal basis. Usually we drop the "op" subscript and allow context to tell whether the Hamiltonian is in matrix or operator representation.

a) Solve by inspection for the eigen-energies and eigenvectors of the initial unperturbed Hamiltonian. To help with the rest of the problem label the states 1, 2, and 3 in some sensible order.

b) Solve for the exact eigen-energies and normalized eigenvectors of the perturbed Hamiltonian: i.e., diagonalize the perturbed Hamiltonian matrix. **HINTS:** It's not so hard—if you don't make a mistake in the first step.

c) Expand the exact eigen-energies and eigenvectors (where applicable) to 2nd order in small ϵ. (Note I mean Taylor expansion, not perturbation series expansion although the two expansion are closely related in this case.) Simplify the eigenvectors to nice forms so that it is easy to see which perturbed vector grew out of which unperturbed vector as ϵ grew from 0.

d) Determine from (weak-coupling) perturbation theory the energies to 2nd order and the eigenvectors to 1st order of the perturbed Hamiltonian. How do these results compare with those of the part (c) answer? **HINT:** Perturbation theory can be applied to the degenerate states in this case because they are completely uncoupled.

e) Now use the truncated Hamiltonian matrix method (or linear variational method if you know it) to find approximate eigen-energies and eigenvectors for the two initially degenerate eigen-energy states. To what order goodness in small ϵ are the results? Why the are results for one perturbed state exact and for the other rather poor compared to the exact results?

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015 qfull 03400 2 3 0 moderate math: variational x**4 potential

19. You are given a 1-dimensional Hamiltonian with a quartic potential:

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0\left(\frac{x}{a}\right)^4 ,$$

where V_0 is a constant. The Hamiltonian applies over the whole x-axis.

a) Write H in a dimensionless form in units of energy $\hbar^2/(2ma^2)$, with $y = x/a$, and with a dimensionless potential constant V_1.

b) Show definitively that a trial Gaussian wave function

$$\psi(x) = Ae^{-\beta x^2/a^2} ,$$

where β is a variational parameter, cannot be an eigenfunction of the Hamiltonian for any value of β. Remember a trial wave function could fortuitously have the right form to be an eigenfunction.

c) Write down the dimensionless variational energy ϵ_{v} using the trial Gaussian wave function and solve for ϵ_{v} as an explicit function of β and V_1. **HINT:** Remember to account for normalization.

d) Sketch ϵ_{v} as a function of β on a schematic plot.

e) Determine the β_{min} value that makes ϵ_{v} stationary and, in fact, a minimum. What is minimum $\epsilon_{\mathrm{v,min}}$? Why can't $\epsilon_{\mathrm{v,min}}$ be the true ground state energy of the dimensionless Hamiltonian? What is the qualitative relation between $\epsilon_{\mathrm{v,min}}$ and $\epsilon_{\mathrm{ground}}$.

Chapt. 16 Variational Principle and Variational Methods

Multiple-Choice Problems

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016 qmult 00700 1 1 3 easy memory: equivalent postulates

1. If two postulates are said to be equivalent, then

   a) one can be derived from the other, but not the other from the one.
   b) the other can be derived from the one, but not the one from the other.
   c) each one can be derived from the other.
   d) neither can be true.
   e) both must be true.

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016 qmult 00800 1 4 5 easy deducto-memory: variational principle

2. "Let's play *Jeopardy*! For \$100, the answer is: Usually the demand that an action (or action integral) be stationary with respect to arbitrary variation in a function appearing somehow in the integrand."

   a) What is a Hermitian conjugate, Alex?
   b) What is an unperturbation principle, Alex?
   c) What is a perturbation principle, Alex?
   d) What is an invariation principle, Alex?
   e) What is a variational principle, Alex?

---

016 qmult 00900 1 1 3 easy memory: quantum mechanics action

3. In non-relativistic quantum mechanics the action of the usual variation principle is:

   a) the integral of angular momentum.
   b) the derivative of angular momentum.
   c) the expectation value of the Hamiltonian.
   d) the time independent Schrödinger equation.
   e) the Dirac equation.

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016 qmult 01000 1 1 1 easy memory: stationary action

4. An exact solution $|\phi\rangle$ to the time-independent Schrödinger equation is the one that by the variational principle in quantum mechanics makes the action

$$E(\phi) = \frac{\langle\phi|H|\phi\rangle}{\langle\phi|\phi\rangle}$$

   be stationary with respect to:

   a) arbitrary variations of the state $|\phi\rangle$ (i.e., $\delta E(\phi) = 0$).
   b) some variations of the state $|\phi\rangle$.
   c) no variations of the state $|\phi\rangle$.
   d) reasonable variations of the state $|\phi\rangle$.
   e) unreasonable variations of the state $|\phi\rangle$.

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016 qmult 01100 1 1 5 easy memory: simple variational method

5. In the simple variational method one takes a parameterized trial wave function and finds the parameters that make the expectation value of the Hamiltonian:

   a) a maximum.
   b) 1.
   c) negative.
   d) positive.
   e) a minimum.

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016 qmult 01200 1 4 3 easy deducto-memory: linear variation method

6. "Let's play *Jeopardy*! For \$100, the answer is: The justification for the linear variational method (or Rayleigh-Ritz method or truncated Hamiltonian matrix eigen-problem)."

   a) What is Hermitian conjugation, Alex?
   b) What is bra/ket notation, Alex?
   c) What is the quantum mechanics variational principle, Alex?
   d) What is the Dirac principle, Alex?
   e) What is the cosmological principle, Alex?

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016 qmult 01500 1 4 1 easy deducto-memory: repulsion of the energy levels

7. Any perturbation applied to a two-level system that is initially degenerate causes:

   a) a repulsion of the energy levels.
   b) an attraction of the energy levels.
   c) a warm and affectionate relationship between the energy levels.
   d) a wonderful, meaningful togetherness of the energy levels.
   e) an eternal soul-bliss of the energy levels.

Full-Answer Problems

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016 qfull 00010 1 5 0 easy thinking: equivalent results

1. If two different looking theorems or postulates were said to be equivalent what would that mean?

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016 qfull 00020 2 5 0 moderate thinking: variational principle and method

2. Are the variational principle and the variational method the same thing? Explain please.

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016 qfull 00030 1 5 0 easy thinking: what is a stationary point?

3. What does it mean to say a function is stationary at a point?

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016 qfull 00040 2 3 0 moderate math: differentiation for stationarity

4. Take the derivative of

$$E(\alpha)=\frac{5}{4}\frac{\hbar^2}{m\alpha^2}+\frac{1}{14}m\omega^2\alpha^2$$

   and determine the stationary point. Just by imagining the function's behavior in the large and small α limits determine whether the stationary point is a minimum. Give the analytic expression for $E(\alpha)$ at the stationary point.

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016 qfull 00050 2 5 0 moderate thinking: Snell's law and var. princ.

5. Can Snell's law be derived using the variational principle (or a variational principle "as you prefer")? Please explain.

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016 qfull 00060 2 5 0 moderate thinking: Schr"od. and var. princ.

6. Can the time-independent Schrödinger's equation be derived using the variational principle? Please explain.

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016 qfull 00070 2 5 0 moderate thinking: convert to matrix eigenproblem

7. Convert the braket eigenproblem $H|\Psi\rangle = E|\Psi\rangle$ to the discrete $\{|u_j\rangle\}$ orthonormal basis representation by expanding $|\Psi\rangle$ in terms of the $|u_j\rangle$ kets and then operating on the equation with the bra $\langle u_i|$. Find the matrix representation of the eigenproblem.

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016 qfull 00080 1 5 0 easy thinking: solving infinite matrix problem

8. Can one literally solve in a numerical procedure an infinite matrix problem: i.e. a problem with an infinite number of terms to number crunch? Why so or why not?

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016 qfull 00090 1 5 0 easy thinking: diagonalization defined

9. What is meant by diagonalization in quantum mechanics?

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016 qfull 00200 2 5 0 moderate thinking: simple variational method

Extra keywords: simple variational method for excited states

10. The simple variational method can in principle be applied to excited states.

    a) Say an unnormalized trial wave function $|\psi\rangle$ is orthogonal to all energy eigenstates $|\phi_i\rangle$ of quantum number less than n, where the eigen-energies increase monotonically with quantum number as usual. Show that $E_{\text{trial}} \geq E_n$ where E_{trial} is the expectation value of the Hamiltonian for $|\psi\rangle$. When will the equality hold? Remember there is such a thing as degeneracy.

    b) Using the simple variational method for finding excited eigenstate energies isn't really of general interest since constructing trial functions with the right orthogonality properties is often harder than using the other approaches. However, if the eigenstates have definite parity, definite parity trial wave functions can be used to determine the lowest eigen-energies for wave functions of each kind of parity.

    For example, let us consider the simple harmonic oscillator problem in one dimension. We know that the eigenstates are non-degenerate and have definite parity. It is given that the ground state has even parity and the first excited state has odd parity. We can use an odd trial wave function and the variational method to approximately determine the energy of the first excited state. The simple harmonic oscillator eigenproblem in scaled dimensionless variables is

$$\left(-\frac{d^2}{dx^2} + x^2\right)\psi = E\psi \ ,$$

where

$$x = \sqrt{\frac{m\omega}{\hbar}}x_{\text{phy}} \qquad \text{and} \qquad E = \frac{E_{\text{phy}}}{\hbar\omega/2} = 2n+1 \ .$$

The n is the SHO energy quantum number (n runs $0, 1, 2, 3, \ldots$) and the "phy" stands for physical. Consider the odd trial wave function

$$\psi = \begin{cases} x(x^2 - c^2), & |x| \leq c; \\ 0. & |x| > c, \end{cases}$$

where c is a variational parameter. Normalize this trial wave function, evaluate its expectation energy, and minimize the expectation energy by varying c. How does this variational method energy compare to the exact result which in scaled variables is 3. **HINT:** There are no wonderful tricks in the integrations: grind them out carefully.

---

016 qfull 00300 3 5 0 tough thinking: variational hydrogen

Extra keywords: (Ha-327:4.1)

11. We know, of course, the ground state for the hydrogenic atom sans perturbations:

$$\psi_{n\ell m} = \frac{1}{\sqrt{4\pi}}(2a^{-3/2})e^{-r/a} \ ,$$

where $a = a_0/[(m/m_e)Z]$ is the radial scale parameter: $a_0 = \hbar^2/(m_e e^2) = \lambda_{\text{Compton}}/(2\pi\alpha) = 0.529\,\text{Å}$ is the Bohr radius, m is the reduced mass, and Z is the nuclear charge (Gr-128, 141). But as a tedious illustration of the simple variational method, let us try find an approximate ground state wave function and energy starting with the trial Gaussian wave function

$$\psi = Ae^{-\beta r^2/a^2} \ .$$

a) Can we obtain the exact solution with a trial wave function of this form?

temitemb) The varied energy is given by

$$E_{\text{v}} = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\int_0^\infty [\psi(r)^* H\psi(r)]\,(4\pi r^2)\,dr}{\int_0^\infty [\psi(r)^*\psi(r)]\,(4\pi r^2)\,dr} \ ,$$

where H is the Hamiltonian for $\ell = 0$ (i.e., the zero angular momentum case) given by

$$H = -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{Ze^2}{r} \ .$$

Note the varied energy form does not require a Lagrange undetermined multiplier since we are building the constraint of normalization into the variation. We, of course, need to evaluate A later to normalize the minimized wave function. Convert the varied energy expression into a dimensionless form in terms of the coordinate $x = r/a$ and reduced varied energy $\epsilon_{\text{v}} = E_{\text{v}}/[Ze^2/(2a)] = Z^{-2}(m/m_e)E_{\text{v}}/E_{\text{Ryd}} \approx Z^{-2}(m/m_e)E_{\text{v}}/(13.606\,\text{eV})$. **HINT:** A further integration transformation can make the analytic form even simpler.

temitemc) Find the explicit analytic expression for ϵ_{v}. Sketch a plot of ϵ_{v} as a function of β. **HINT:** Use an integral table.

d) Now find the minimizing β value and the minimum ϵ_{v}. Compare ϵ_{v} to exact ground state value which is -1 in fact.

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016 qfull 01000 3 5 0 tough thinking: non-orthogonal linear variation

Extra keywords: method for a two level system.

12. You are given two basis states $|1\rangle$ and $|2\rangle$ and want to solve a two-dimensional system with Hamiltonian H in terms of this basis. The basis is not orthogonal although the basis states are normalized of course. Recall in this case that the non-orthogonal linear variational method eigenproblem is

$$H\vec{c} = ES\vec{c} \ ,$$

where $\vec{c}$ is an unknown eigenvector, E and unknown eigen-energy, and S is the overlap matrix.

Let

$$H = \begin{pmatrix} \varepsilon_1 & V \\ V & \varepsilon_2 \end{pmatrix} \ .$$

We have assumed that $\langle 1|H|2\rangle = \langle 2|H|1\rangle$ and designated these elements by V: i.e., the eigenstates are pure real. This assumption is generality that probably pointless for the cases where this problem is probably of most interest: i.e., in LCAO method (i.e., linear combination of atomic orbitals method) for molecular orbitals. We will also assume $V < 0$ which is also appropriate for LCAO, and so avoids needles generality. As a fiducial choice assume $\varepsilon_2 \geq \varepsilon_1$ although all the formulae will not depend this choice in fact. For the overlap matrix let

$$S = \begin{pmatrix} \langle 1|1\rangle & \langle 1|2\rangle \\ \langle 2|1\rangle & \langle 2|2\rangle \end{pmatrix} = \begin{pmatrix} 1 & s \\ s & 1 \end{pmatrix} .$$

Your mission Mr. Phelps—if you choose to accept it—is solve for the eigen-energies and eigenvectors. These quantities tend to come out in clumsy forms. So you should try to find nice forms. You may subsume large clumpy expressions into single symbols, but show some restraint. One trick is to re-origin all the energies: i.e., define

$$\bar{\varepsilon} = \frac{\varepsilon_1 + \varepsilon_2}{2} , \qquad -\varepsilon' = \varepsilon_1 - \bar{\varepsilon} , \qquad \varepsilon' = \varepsilon_2 - \bar{\varepsilon} , \qquad V' = V - \bar{\varepsilon} s , \qquad \text{and} \qquad E' = E - \bar{\varepsilon} .$$

Note with our fiducial assumptions $\varepsilon' \geq 0$, but all the formula should work for $\varepsilon' < 0$ too. Note also that $V' < 0$, $V' > 0$, or $V' = 0$ are all possible now. Now subtract

$$\bar{\varepsilon} \begin{pmatrix} 1 & s \\ s & 1 \end{pmatrix} \vec{c}$$

from both sides of the eigenproblem and solve for the primed eigen-energies and the eigenvectors in terms of the primed quantities. Having found the solutions, you should examine the special limiting cases: i.e., $\varepsilon' \to 0$, and $s \to 0$.

The State Department confesses that it does not know the ideal forms for the solutions and in any case will disavow all knowledge of your activities.

Chapt. 17 Time-Dependent Perturbation Theory

Multiple-Choice Problems

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017 qmult 00100 1 1 4 easy memory: Fermi, person identification
Extra keywords: Fermi, person identification

1. Who was Enrico Fermi?

   a) An Italian who discovered America in 1492.
   b) An Italian who did not discover America in 1492.
   c) An Italian-American biologist.
   d) An Italian-American physicist.
   e) Author of *Atoms in the Family*.

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017 qmult 00200 1 4 5 easy deducto-memory: golden rule
Extra keywords: Sc-288

2. "Let's play *Jeopardy*! For \$100, the answer is: This quantum mechanical time-dependent perturbation result was discovered by Pauli, but named by Fermi."

   a) What is the categorical imperative, Alex?
   b) What is the sixth commandment, Alex?
   c) What is the no-fault insurance, Alex?
   d) What is the iron law, Alex?
   e) What is the golden rule, Alex?

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017 qmult 00300 1 4 5 easy deducto-memory: golden rule validity

3. "Let's play *Jeopardy*! For \$100, the answer is: This aureate time-dependent perturbation result requires, among other things, that

$$\delta E_{\text{level separation}} << \frac{2\pi\hbar}{t - t_{\text{char}}} \lesssim \Delta E_{\text{bandwidth}} ,$$

   where $\delta E_{\text{level separation}}$ is of order of the separation between energy levels in a continuum band of energy levels, $t - t_{\text{char}}$ is the time since the perturbation became significant (i.e., t_{char}), and $\Delta E_{\text{bandwidth}}$ is the characteristic energy width of the continuum band."

   a) What is 2nd order perturbation, Alex?
   b) What is 3rd order perturbation, Alex?
   c) What is the optical theorem, Alex?
   d) What is Pauli's exclusion principle, Alex?
   e) What is Fermi's golden rule, Alex?

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017 qmult 00100 1 1 4 easy memory: exponential decay of state

4. Fermi's golden rule if it applies to transitions to all states from an original state and for all time after a perturbation is applied (which may be from the time the original state forms) causes the original state to have:

   a) no transitions.

b) a linear decline in survival probability.
c) a power law decline in survival probability.
d) an exponential decline in survival probability.
e) an instantaneous decline in survival probability.

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017 qmult 00800 1 1 5 easy memory: harmonic perturbation, sinusoidal

Extra keywords: harmonic perturbation, sinusoidal time dependence

5. Harmonic perturbations have:

a) a linear time dependence.
b) a quadratic time dependence.
c) an inverse time dependence.
d) an exponential time dependence.
e) a sinusoidal time dependence.

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017 qmult 01200 1 1 1 easy memory: principal value integral

6. One can sometimes in integrate over a first order singularity and get a physically reasonable result. This kind of integral is called:

a) a principal value integral or Cauchy principal value integral.
b) an interest integral.
c) a capitol integral.
d) a bull-market integral.
e) a bear-market integral.

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017 qmult 02000 1 1 5 easy memory: electric dipole selection rules

Extra keywords: electric dipole selection rules

7. The selection rules for electric dipole transitions are:

a) $\Delta l = 0$ and $\Delta m = 0$.
b) $\Delta l = \pm 2$ and $\Delta m = \pm 1$.
c) $\Delta l = -1$ and $\Delta m = 1$.
d) $\Delta l = \pm 1$ and $\Delta m = 0$.
e) $\Delta l = \pm 1$ and $\Delta m = 0,\ \pm 1$.

Full-Answer Problems

017 qfull 00010 1 5 0 easy thinking: time-dependent Sch.eqn.

1. Is the time-dependent Schrödinger equation needed for time-dependent perturbation theory?

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017 qfull 00020 2 5 0 moderate thinking: energy eigenstates

2. Are stationary states (i.e., energy eigenstates) needed in time-dependent perturbation theory? Please explain.

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017 qfull 00030 2 5 0 moderate thinking: energy eigenstates

3. What is done with the radiation field in quantum electrodynamics.

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017 qfull 00100 2 3 0 easy math: Fermi's golden rule integral

Extra keywords: Fermi's golden rule integral, Simpson's rule

4. In the simplest version of the derivation of Fermi's golden rule one uses the integral

$$\int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2}\,dx = \pi$$

which can be evaluated using complex variable contour integration (Ar-364). One of the features of this integral that is used in the justification of the golden rule is that most of the total comes from the central bump of the integrand: i.e., the region $[-\pi,\pi]$. It would be good to know what fraction of the total comes from the central bump. Alas,

$$I_{\text{cen}}=\int_{-\pi}^{\pi}\frac{\sin^2 x}{x^2}\,dx\ .$$

is not analytically solvable.

a) Find an excellent approximate value for I_{cen}. **HINTS:** It's probably no good trying to find a good approximation for the central bump directly since it is most of the total. An approximate value could easily turn out to be off by of order $|I_{\text{cen}}-\pi|$. Try finding a value for the non-central bump region.

b) Now—if you dare—evaluate I_{cen} numerically and compare to your analytic result from part (a). **HINT:** I use double precision Simpson's rule myself.

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017 qfull 00200 3 3 0 tough math: time dependent perturbation, square well

Extra keywords: (MEL-141:5.3), time dependent perturbation, infinite square well

5. At time $t=0$, an electron of charge $\tilde e$ is in the n eigenstate of an infinite square well with potential

$$V(x)=\begin{cases}0, & x\in[0,a];\\ \infty & x>a.\end{cases}$$

At that time, a constant electric field $\tilde E$ pointed in the positive x direction is suddenly applied. (Note the tildes on charge and electric field are to distinguish these quantities from the natural log base and energy.) **NOTE:** The 1-d infinite square-well eigenfunctions and eigen-energies are, respectively

$$\psi_n(x)=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)\qquad\text{and}\qquad E_n=\frac{\hbar^2k^2}{2m}=\frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2n^2\ ,$$

where $n=1,2,3,\ldots$ The sinusoidal eigenfunctions can be expressed as exponentials: let $z=\pi x/a$, and then

$$\sin(nz)=\frac{e^{inz}-e^{-inz}}{2i}\ .$$

a) Use 1st order time-dependent perturbation theory to calculate the transition probabilities to all **OTHER** states m as a function of time. You should evaluate the matrix elements as explicitly: this is where all the work is naturally.

b) How do the transition probabilities vary with the energy separation between states n and m?

c) Now what is the 1st order probability of staying in the same state n?

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017 qfull 00300 3 5 0 tough thinking: usual and general Fermi's golden rule

6. Say we have time-dependent perturbation

$$H(t)=\begin{cases}0, & t<0;\\ H, & t\geq 0,\end{cases}$$

and initial state $|\phi_j\rangle$, where $|\phi_j\rangle$ is the eigenstate belonging to the complete set $\{|\phi_i\rangle\}$. The state at any time $t\geq 0$ is $|\Psi(t)\rangle$.

a) Work out as far as one reasonably can the 1st order perturbation expression for the coefficient $a_i(t)$ in the expansion of $|\Psi(t)\rangle$ in terms of the set $\{|\phi_i\rangle\}$. Include the case of $i = j$. **HINT:** The worked out expression should contain a sine function. Define $\omega_{ij} = (E_i - E_j)/\hbar$.

b) Given $i \neq j$, find the transition probability (to 1st order of course) from state j to state i.

c) What is this probability at early times when $\omega_{ij}t/2 << 1$ for all possible ω_{ij}? Describe the behavior of the probability as a function of time for all times. (You could sketch a plot of probability as a function of time.) What is the behavior for $\omega_{ij} = 0$ (i.e., for transitions to degenerate states)?

d) You want to calculate the summed probability of transition to some set of states (which may not be all possible states) that are dense enough in energy space to form a quasi-continuum or even a real continuum of states. The set does not include the initial state j. The summed probability for energy interval E_a to E_b can be approximated by an integral:

$$P(t) = \sum_{i \neq j} P_i(t) \approx \int_{E_a}^{E_b} P(E,t)\rho(E)\,dE \ ,$$

where $\rho(E)$ is the density of states per unit energy and where the time-independent part of the matrix element H_{ij} is replaced by $H(E)$ which is a continuous function of energy.

What is the total transition probability to all states in the set assuming integrand is only significant in small region near E_j. The region is small eneough that $|H(E)|^2$ and $\rho(E)$ can be taken as constants and that the limits of integration can be set to $\pm\infty$. (Note you will probably need to look up a standard definite integral.)

In fact, 90 % of the integral (assuming $|H(E)|^2$ and $\rho(E)$ constant) comes from the energy range $[E_j - 2\pi\hbar/t, E_j + 2\pi\hbar/t]$. (Can you show this by a numerical integration? No extra credit for doing this: insight is the only reward.) We can see that at some time the 90 %-range will be so narrow that the approximation $|H(E)|^2$ and $\rho(E)$ constant will probably become valid. They should clearly be evaluated at E_j. Practically, this often means that the approximation becomes valid when almost all of the transitions are to nearly degenerate states. Of course, the 90 %-range can become so narrow that the approximation of a continuum of states breaks down and then the integration becomes invalid again. In fact, for the integration to be valid we require $|H(E)|^2$ and $\rho(E)$ to be constant over ΔE such that $\Delta E \gtrsim 2\pi\hbar/t$ and that the energy separation δE between the final satisfy $\delta E << 2\pi\hbar/t$. Thus we require

$$\delta E << 2\pi\hbar/t \lesssim \Delta E \ .$$

What is the rate of transition for (i.e., time derivative of) the total transition probability? The transition rate result is one of the usual forms of Fermi's golden rule. Although it is restricted in many ways, it is still a very useful result: hence golden.

e) Let's see if we can derive a generalized golden rule without the restriction that the perturbation is constant after a sudden turn-on. To do this assume that the perturbation Hamiltonian has the form

$$H(t) = Hf(t) \ ,$$

where H is now constant with time and $f(t)$ is a real turn-on function with the property that $f(t)$ is significant only for $t \geq t_{\text{ch}}$, where t_{ch} is a characteristic time for turn-on. Let time zero be formally set to $-\infty$ for generality.

First, derive $P_i(t)$ with explicit integrals. Second, assume again that there is a continuum or quazi-continuum of states (of which state i is one) with density of states $\rho(E)$ and that H_{ij}

can be replaced by $H(E)$. Third, argue that the time integrals must be sharply peaked functions of E about the initial $E = E_j$ for $t \geq t_{\rm ch}$. Fourth, re-arrange the integrals and integrate over energy making use of the third point. You can then make use of the result

$$\delta(x) = \int_{-\infty}^{\infty} \frac{e^{\pm ikx}}{2\pi}\, dk \ ,$$

where $\delta(x)$ is the Dirac delta function (Ar-679). What is the total transition probability for $t \geq t_{\rm ch}$? What is the total transition rate $t \geq t_{\rm ch}$? When does this generalized golden rule reduce to Fermi's golden rule?

Chapt. 18 The Hydrogenic Atom and Spin

Multiple-Choice Problems

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018 qmult 00100 1 1 4 easy memory: spin-orbit interaction, hydrogenic atom

Extra keywords: spin-orbit interaction, hydrogenic atom

1. What is the main internal perturbation/perturbations preventing the spinless hydrogenic eigenstates from being the actual ones?

   a) The Stark effect. b) The Zeeman effect. c) The Stern-Gerlach effect.
   d) The spin-orbit interaction and the relativistic perturbation.
   e) The Goldhaber interaction.

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018 qmult 00200 2 4 5 moderate deducto-memory: orbital ang. mom., spin

Extra keywords: orbital angular momentum, spin, total angular momentum

2. The scalar product of operators $\vec{L}\cdot\vec{S}$ equals

   a) J^2.
   b) $(\vec{L}+\vec{S})\cdot(\vec{L}+\vec{S})$.
   c) $(\vec{L}-\vec{S})\cdot(\vec{L}-\vec{S})$.
   d) $(J^2+L^2+S^2)/2$.
   e) $(J^2-L^2-S^2)/2$.

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018 qmult 00300 1 4 3 easy deducto-memory: spin-orbit good quantum numbers

Extra keywords: spin-orbit interaction, good quantum numbers

3. "Let's play *Jeopardy*! For $100, the answer is: The spin-orbit interaction causes the eigenstates of the real hydrogen atom to be mixtures of the $\Psi_{n\ell m}$ states, but one $\Psi_{n\ell m}$ state is usually overwhelmingly dominant.

   a) Why are the quantum numbers n, ℓ, and m perfectly rotten, Alex?
   b) Why are the quantum numbers n, ℓ, and m only approximately rotten, Alex?
   c) Why are the quantum numbers n, ℓ, and m only approximately good, Alex?
   d) Why are the quantum numbers n, ℓ, and m only indifferent, Alex?
   d) Why are the quantum numbers n, ℓ, and m dependent on a recount in Palm Beach, Alex?

Full-Answer Problems

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018 qfull 00500 1 3 0 easy math: fine-structure energy levels

1. The hydrogen atom energy level energies corrected for the fine structure perturbations (i.e., the relativistic and spin-orbit perturbations) is

$$E(n,\ell,\pm 1/2,j) = -\frac{E_{\rm Ryd}}{n^2}\frac{m}{m_e}\left[1+\frac{\alpha^2}{n^2}\left(\frac{n}{j+1/2}-\frac{3}{4}\right)\right] ,$$

where n is the principal quantum number, ℓ is the orbital angular momentum quantum number, $\pm 1/2$ is allowed variations of j from ℓ, j (the total angular momentum quantum number) is a redundant parameter since $j = \max(\ell \pm 1/2, 1/2)$ (but it is a convenient one),

$$E_{\text{Ryd}} = \frac{1}{2} m_e c^2 \alpha^2$$

is the Rydberg energy, m_e is the electron mass, $\alpha \approx 1/137$ is the fine structure constant, and

$$m = \frac{m_e m_p}{m_e + m_p}$$

is the reduced mass with m_p being the proton mass. The bracketed perturbation correction term is

$$\frac{\alpha^2}{n^2} \left(\frac{n}{j + 1/2} - \frac{3}{4} \right)$$

which is of order $\alpha^2 \approx 10^{-4}$ times smaller than the unperturbed energy. Show that the perturbation term is always negative and reduces the energy from the unperturbed energy: i.e., show that

$$\frac{n}{j + 1/2} - \frac{3}{4} > 0$$

in all cases.

Chapt. 19 Symmetrization Principle

Multiple-Choice Problems

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019 qmult 00100 1 4 5 easy deducto-memory: symmetrization principle

1. "Let's play *Jeopardy*! For $100, the answer is: It is the quantum mechanics **POSTULATE** that the state for identical fundamental particles must be symmetrized: i.e., must be symmetric or antisymmetric under the exchange of any two particles in the state expression. Bosons have symmetric state and fermions antisymmetric states. A second part of the postulate is that integer spin particles are bosons and half-integer spin particles are fermions. The postulate evolved in the 1920s from the work of Pauli, Fierz, Weisskopf, Heisenberg, Dirac, and others: there seems to be no one discoverer. An immediate corollary of the postulate is that composite particles with identical constituent elementary particles obey the postulates too even though the composite particles are not identical in their states because of excitations and perturbations. The composite particles are identical in their properties (though not their state), and so are called identical too. A composite particle is boson if it contains an even number of fermions and a fermion if it contains an odd number of fermions.

   Actually one needs to define exchange. A general definition is too much for here. For simplicity, we will only consider two particles whose state is given in the spatial representation: i.e., by a wave function. The formalism (justifed by it working) is to give each particle its own spatial coordinate and spin coordinate. Particle 1 has coordinate set $\vec{r}_1 m_1$ and particle 2 has coordinate set $\vec{r}_2 m_2$. The state of the system is the wave function

   $$\psi(\vec{r}_1 m_1, \vec{r}_2 m_2) \ .$$

   In general, the function will have a different dependence on the two coordinate sets. If we exchange we get the new state

   $$\psi_{\text{new}}(\vec{r}_1 m_1, \vec{r}_2 m_2) = \psi(\vec{r}_2 m_2, \vec{r}_1 m_1) \ .$$

   In quatnum mechanics jargon, the coordinate set exchange is called exchanging the particles. The new state is clearly in general a different mathematical state of the formal coordinate sets. The new state will be the same mathematically as the old state only if it is symmetric: i.e., only if

   $$\psi(\vec{r}_2 m_2, \vec{r}_1 m_1) = \psi(\vec{r}_1 m_1, \vec{r}_2 m_2)$$

   for all values of the coordinate sets.

   If the particles are physically distinct, we create in general a different state by particle exchange. This is because the new state will evolve differently in time in general because the distinct particles are affected by different potentials in general. Note that the two particles do have to have the same spin for the exchange to be mathematically and physically consistent. The only way the new state could be the same physical state as the original state is if

   $$\psi(\vec{r}_2 m_2, \vec{r}_1 m_1) = e^{i\phi}\psi(\vec{r}_1 m_1, \vec{r}_2 m_2) \ ,$$

   where ϕ is a constant phase factor. A constant phase factor does not change the physical state though, of course, it changes the mathematical state.

If the two particles are identical, then particle exchange creates clearly does not create a different physical state even though it creates a different mathematical state. But this causes a paradox which is called the exchange paradox. A linear combination state

$$\psi_{\rm com}(\vec r_1 m_1,\vec r_2 m_2)=c_i\psi(\vec r_1 m_1,\vec r_2 m_2)+c_j\psi(\vec r_2 m_2,\vec r_1 m_1)$$

is mathematically and, a priori, physically distince from $\psi(\vec r_1 m_1,\vec r_2 m_2)$. The coefficients c_i and c_j are only constrained, a priori, by the requirement that $\psi_{\rm com}(\vec r_1 m_1,\vec r_2 m_2)$ be normalized. In quantum mechanics, $\psi_{\rm com}(\vec r_1 m_1,\vec r_2 m_2)$ describes the system in a superposition of states $\psi(\vec r_1 m_1,\vec r_2 m_2)$ and $\psi(\vec r_2 m_2,\vec r_1 m_1)$. But how can an infinite continuum of distinct states be created by the superposition of a state with itself. The paradox has no derivable solution. It is resolved by the postulate we are describing.

To see the resolution, say that state $\psi(\vec r_1 m_1,\vec r_2 m_2)$ has the general exchange property that

$$\psi(\vec r_2,\vec r_1)=e^{i\phi}\psi(\vec r_1,\vec r_2)\ .$$

Now the linear combination state

$$\begin{aligned}\psi_{\rm com}(\vec r_1 m_1,\vec r_2 m_2)&=c_i\psi(\vec r_1 m_1,\vec r_2 m_2)+c_j\psi(\vec r_2 m_2,\vec r_1 m_1)\\&=c_i\psi(\vec r_1 m_1,\vec r_2 m_2)+c_je^{i\phi}\psi(\vec r_1 m_1,\vec r_2 m_2)\\&=(c_i+c_je^{i\phi})\psi(\vec r_1 m_1,\vec r_2 m_2)\end{aligned}$$

which is physically the same state as before: mathematically it differs by a constant phase factor. The general exchange property resolves the exchange paradox. But what sets the phase factor $e^{i\phi}$. Arguments we will not go into here suggest that only $e^{i\phi}=\pm1$ are reasonable phase factor values. Observation tells us that $e^{i\phi}=1$ holds for integer spin particles and $e^{i\phi}=-1$ holds for half-integer spin particles. This observation becomes part of the postulate we are describing. Actually, the spin-statistics theorem proves the spin rule, but that theorem itself depends on hypotheses which may not be true (CT-1387). Also actually quasiparticles called anyons that exist in two-dimensional systems have the general exchange property rather than just the $e^{i\phi}=\pm1$ possibilities."

What is ____________, Alex?

a) Born's hypothesis b) Schrödinger's dilemma c) Dirac's paradox
d) Wigner's last stand e) the symmetrization principle or postulate

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019 qmult 00110 1 1 3 easy memory: exchange degeneracy and symmetrization principle

2. As strange as the symmetrization principle seems at first, quantum mechanics would be inconsistent without it since then you could create infinitely many physically distinct states by superpositions of the same state. This inconsistency is called the:

a) symmetrization paradox. b) symmetrization degeneracy.
c) exhcange degeneracy. d) baffling degeneracy. e) baffling paradox.

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019 qmult 01000 1 4 5 easy deducto-memory: Bose-Einstein condensate

Extra keywords: References Gr-216, CT-1399, Pa-179

3. "Let's play *Jeopardy*! For $100, the answer is: The name for the state of a system of all identical bosons when all the bosons or at least a large fraction settle into the ground state."

What is ____________, Alex?

a) a Hermitian conjugate b) a Hermitian condensate
c) a Rabi-Schwinger-Baym-Sutherland-Jeffery degeneracy d) just another state
e) a Bose-Einstein condensate

Full-Answer Problems

019 qfull 00100 2 5 0 moderate thinking: permutation operator

1. The permutation operator P for functions of two variables has the seemingly arbitrary, but well defined, property that

$$Pf(x_1,x_2)=f(x_2,x_1)\ ,$$

where $f(x_1,x_2)$ is a general complex function of two real number variables or, one could say, coordinates. Note that an operator is formally a mathematical entity that changes a function into another function or, in a more general context, changes a generalized vector into another generalized vector. Thus $Pf(x_1,x_2)$ is **NOT** $f(x_1,x_2)$ evaluated with exchanged argument values, but a new function of coordinates x_1 and x_2 that has values equal to $f(x_2,x_1)$. Of course, if one views x_1 and x_2 as just particular values and not coordinates, then one can view $Pf(x_1,x_2)$ just as $f(x_1,x_2)$ evaluated with exchanged argument values—but that's not the way we view things in this question.

a) Say x_1 and x_2 are orthogonal coordinates with the x_2 counterclockwise from the x_1. Describe $Pf(x_1,x_2)$ in comparison to $f(x_1,x_2)$. **HINT:** It might be helpful to consider specific points in the x_1-x_2 plane (a,b) and (b,a) which are obviously mirror reflection positions relative to each other about the $x_1=x_2$ line.

b) Prove that P is a linear operator: i.e., that

$$P[f(x_1,x_2)+g(x_1,x_2)]=Pf(x_1,x_2)+Pg(x_1,x_2)]\ .$$

HINT: Define

$$h(x_1,x_2)=f(x_1,x_2)+g(x_1,x_2)\ .$$

c) What is

$$P\left[\frac{\partial f(x_1,x_2)}{\partial x_1}\right]$$

equal to. **HINT:** You might consider a specific example first, e.g., one with

$$f(x_1,x_2)=x_1^3x_2\ .$$

But for a general proof, recall the definition of the derivative

$$\frac{df(x)}{dx}=\lim_{h\to0}\frac{f(x+h)-f(x)}{h}\ .$$

d) Show that the permutation operation and the complex conjugation operation commute: i.e., show that

$$[Pf(x_1,x_2)]^*=P\left[f(x_1,x_2)^*\right]\ .$$

HINT: Decompose $f(x_1,x_2)$ into real and imaginary parts.

e) Show from the definition of the Hermitian conjugate,

$$\langle\phi|Q|\psi\rangle=\langle\psi|Q^\dagger|\phi\rangle^*$$

(where Q is any operator), that P is a Hermitian operator: i.e., that $P=P^\dagger$. **HINT:** Recall that for two spatial dimensions

$$\langle\phi|Q|\psi\rangle=\int_1\int_2\phi(x_1,x_2)^*Q\psi(x_1,x_2)\,dx_1\,dx_2\ .$$

f) Solve for **ALL** the eigenvalues of P.

g) Show that any function $f(x_1, x_2)$ can be expanded in eigenfunctions of P, and thus the eigenfunctions of P form a complete set for the space of functions of two coordinates including wave function spaces of two coordinates. Show explicitly that the eigenfunctions of different eigenvalues are orthogonal. Since P is Hermitian and has a complete set of eigenfunctions for any wave function space of two arguments, it is formally a quantum mechanical observable.

h) Given that $A(x_1, x_2)$ is an operator, show that

$$PA(x_1, x_2)f(x_1, x_2) = A(x_2, x_1)Pf(x_1, x_2) \ ,$$

where $A(x_2, x_1)$ could be a function operator, a differentiating operator or both. Recall that operators act on everything to the right—except, of course, when they don't: but that situation is usually (but not always) made explicit with brackets. Do P and A commute in general? When do they commute?

i) Show that P and the Hamiltonian for identical particles,

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2} + V(x_1, x_2) \ ,$$

commute. Show that if $\psi(x_1, x_2)$ is an eigenstate of the Hamiltonian, then $P\psi(x_1, x_2)$ is an eigenstate. If $\psi(x_1, x_2)$ is non-degenerate in energy, is $P\psi(x_1, x_2)$ a physically distinct state? Show that there are only two possibilities for what $P\psi(x_1, x_2)$ is?

j) Given that P and H commute, show that P is a constant of the motion as far as Schrödinger equation evolution goes.

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019 qfull 00200 1 3 0 easy math: symmetrization principle

2. Consider the general normalized wave function for two particles

$$\Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)$$

where $\vec{r}$ is the spatial coordinate, m is the spin coordinate, and the labels 1 and 2 are formally assigned to particles 1 and 2.

a) First, let's assume that the two particles are physically distinct. This means that under some circumstances, but not all in general, they we behave differently. Say we now act on the state with the permutation operator $P_{2,1}$ and obtain

$$P_{2,1}\Psi(\vec{r}_1 m_1, \vec{r}_2 m_2) = \Psi(\vec{r}_2 m_2, \vec{r}_1 m_1) = \pm\Psi(\vec{r}_1 m_1, \vec{r}_2 m_2) \ ,$$

where we recall that the two-particle permutation operator is Hermitian and only has eigenvalues ±1. Have we created a new physical state? Explain. Say we now act on the state with the permutation operator $P_{2,1}$

$$P_{2,1}\Psi(\vec{r}_1 m_1, \vec{r}_2 m_2) = \Psi(\vec{r}_2 m_2, \vec{r}_1 m_1) \neq \pm\Psi(\vec{r}_1 m_1, \vec{r}_2 m_2) \ .$$

Have we created a new physical state? Explain.

b) Now let's say that the two particles are identical and

$$P_{2,1}\Psi(\vec{r}_1 m_1, \vec{r}_2 m_2) = \Psi(\vec{r}_2 m_2, \vec{r}_1 m_1) \neq \pm\Psi(\vec{r}_1 m_1, \vec{r}_2 m_2) \ ,$$

where we recall that the two-particle permutation operator is Hermitian and only has eigenvalues ±1. Have we created a physically distinct state? Explain. (For the moment, we are not assuming the symmetrization principle.)

c) Carrying over the assumptions of part (b), consider the mixed state

$$\Psi_{\text{mixed}} = c_i\Psi(\vec{r}_1m_1,\vec{r}_2m_2) + c_j\Psi(\vec{r}_2m_2,\vec{r}_1m_1) \ ,$$

where the only constraint on coefficients c_i and c_j is the the normalization constraint coefficients c_i and c_j

$$|c_i|^1 + |c_j|^2 + \text{Re}[c_ic_j\langle\Psi(\vec{r}_1m_1,\vec{r}_2m_2)|\Psi(\vec{r}_2m_2,\vec{r}_1m_1)\rangle] = 1 \ .$$

Note we are not assuming $\Psi(\vec{r}_1m_1,\vec{r}_2m_2)$ and $P_{21}\Psi(\vec{r}_1m_1,\vec{r}_2m_2)$ are orthogonal.

Argue that Ψ_{mixed} is physically distinct from $\Psi(\vec{r}_1m_1,\vec{r}_2m_2)$ and $P_{21}\Psi(\vec{r}_1m_1,\vec{r}_2m_2)$?

Actually, there is a continuum infinity of possible Ψ_{mixed} which is only constrained by the normalization constraint. This infinity of states that can be constructed from $\Psi(\vec{r}_1m_1,\vec{r}_2m_2)$ and $P_{21}\Psi(\vec{r}_1m_1,\vec{r}_2m_2)$ is called the exchange degeneracy (CT-1375).

Given the widely, but not universally, accepted quantum mechanical interpretation, that a linear combination of states constitutes a particle or a set of particles in a superposition of those states argue that the exchange degeneracy creates a paradox.

d) The paradox of part (c) is eliminated by invoking the symmetrization principle that states that the only physically allowed state for a set of identical particles is one that is symmetrized: i.e., is one that is symmetric (i.e., an eigenstate of the permutation operator with eigenvalue 1) or antisymmetric (i.e., an eigenstate of the permutation operator with eigenvalue -1) under the exchange of any pair of particles. Note identical particles of one type can have only one kind of symmetrized wave functions: i.e., they must either have only symmetric ones in all cases (in which case they are called bosons) or only antisymmetric ones in all cases (in which case they are called fermions). A separate postulate or if one prefers an extra part of the symmetrization principle is that integer-spin particles are bosons and half-integer-spin particles are fermions. Explain how the symmetrization principle eliminated the paradox.

e) The Hamiltonian for a set of identical particles is necessarily symmetric. What does this imply for the symmetrization state of the state as time passes?

f) Say that you had a set of non-identical particles that in a certain system had a symmetric Hamiltonian. Say the particles were put into a symmetrized state. Would the state stay symmetrized as time passes?

g) The symmetrization principle can be taken as stated for fundamental particles only. But it applies as an immediate corollary to identical composite particles where whether particle is boson or fermion depends on whether it contains an even or odd number of fermions. Prove the corollary.

h) The Pauli exclusion principle is actually a corollary of the symmetrization principle. One version is that the probability amplitude and therefore probability of density for two identical fundamental fermions at the spatial coordinate and spin coordinate is zero. Prove this.

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019 qfull 00210 2 5 0 moderate thinking: exchange degeneracy

Extra keywords: Probably absolutely displaced now by 00200

3. Say you have two distinct, **ORTHONORMAL** single-particle energy eigenstates $\psi_a(x)$ and $\psi_b(x)$ and you wish to construct from them a two-particle energy eigenstate for two identical spinless particles: particles 1 and 2. One possibility is

$$\psi(x_1,x_2) = \psi_a(x_1)\psi_b(x_2) \ .$$

A more general two-particle state is

$$\psi(x_1,x_2)=c_1\psi_a(x_1)\psi_b(x_2)+c_2\psi_a(x_2)\psi_b(x_1)\ .$$

NOTE: We are only discussing spatial eigenstates here, not full time dependent wave functions.

a) Find the condition on the coefficients c_1 and c_2 such that $\psi(x_1,x_2)$ is normalized.

b) How many energy degenerate states can be formed by the various choices of c_1 and c_2 consistent with normalization? This degeneracy is called the exchange degeneracy (CT-1376). Would this degeneracy exist if the particles were distinct? Why or why not?

c) All of statistical mechanics and atomic spectroscopy (where transition rates depend on degeneracies) tell us that the vast degeneracy found in the part (b) answer does not exist in nature. No limitation on this degeneracy can be derived. But one can postulate a limitation. Given that the particles are identical, one natural way to mostly kill the degeneracy is to postulate that the only allowed choices of c_1 and c_2 are those that yield the same expectation value for an observable that formally depends only one particle's coordinate no matter which particle coordinate is used. To be more explicit, say observable Q_1 and Q_2 are identical, except that Q_1 depends only on x_1 and Q_2 depends only on x_2. Solve for c_1 and c_2, such that in general

$$\langle Q_1\rangle=\langle Q_2\rangle\ .$$

HINT: Don't forget the cross terms. Also note that c_1 and c_2 pairs that only differ by a common phase factor are not physically distinct since wave functions that differ only by a global phase factor are actually only one physical wave function.

d) Evaluate $\langle x_1\rangle$ and $\langle x_2\rangle$ for the allowed c_1 and c_2 values found in the part (c) answer. You can take as given

$$\langle x\rangle_a=\langle\psi_a|x|\psi_a\rangle\qquad\text{and}\qquad\langle x\rangle_b=\langle\psi_b|x|\psi_b\rangle\ .$$

Formally the operators x_1 and x_2 are quantum mechanical observables. But would the expectation values $\langle x_1\rangle$ and $\langle x_2\rangle$ be **INDIVIDUALLY** observable in fact if for c_1 and c_2 values other than those allowed by the part (c) answer?

e) Show that the wave functions with the allowed coefficients are eigenfunctions of the permutation operator P which has the effect on the wave function that

$$P\psi(x_1,x_2)=\psi(x_2,x_1)\ .$$

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019 qfull 02000 2 5 0 moderate thinking: symmetrization of 4 orthonormal single-particle states

Extra keywords: defect in part (b). Must rework.

4. Say $|ai\rangle$ and $|bi\rangle$ are **ORTHONORMAL** single-particle states, where i is a particle label. The label can be thought of as labeling the coordinates to be integrated or summed over in an inner product: see below. The symbolic combination of such states for two particles, one in a and one in b is

$$|12\rangle=|a1\rangle|b2\rangle\ ,$$

where 1 and 2 are particle labels. This combination is actually a tensor product, but let's not worry about that now. The inner product of such a combined state is written

$$\langle 12|12\rangle=\langle a1|a1\rangle\langle b2|b2\rangle\ .$$

If one expanded the inner product in the position and spinor representation assuming the wave function and spinor parts can be separated (which in general is not the case),

$$\langle 12|12\rangle = \left[\int \psi_a(x_1)^*\psi_a(x_1)\,dx_1\,(\,c_{a+}^* \quad c_{a-}^*\,)_1 \begin{pmatrix} c_{a+} \\ c_{a-} \end{pmatrix}_1\right] \times \left[\int \psi_b(x_2)^*\psi_b(x_2)\,dx_2\,(\,c_{b+}^* \quad c_{b-}^*\,)_2 \begin{pmatrix} c_{b+} \\ c_{b-} \end{pmatrix}_2\right] .$$

A lot of conventions go into the last expression: don't worry too much about them.

a) Let particles 1 and 2 be distinct particles. What are the two normalizaed product 2-particle states that can be constructed from states a and b? What happens if $a = b$ (i.e., the two single-particle states are only one state actually)?

b) Say particles 1 and 2 are identical bosons or identical fermions. What is the only normalized physical 2-particle state that can be constructed in either case allowing for the possibility that $a = b$ (i.e., the two single-particle states are only one state actually)? What happens to the state if $a = b$ for bosons and what does it mean? What happens to the state if $a = b$ for fermions and what does it mean?

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019 qfull 02100 1 5 0 easy thinking: slater determinant, triplet singlet
Extra keywords: (Gr-181:5.3)

5. Say that we have obtained four distinct orthonormal single-particle eigenstates for identical spin 1/2 particles:

$$\psi_a(\vec r\,)\chi_+ \;, \qquad \psi_a(\vec r\,)\chi_- \;, \qquad \psi_b(\vec r\,)\chi_+ \;, \qquad \psi_b(\vec r\,)\chi_- \;,$$

where the spinors are

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{and} \qquad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix} .$$

To label a state for a particular particle i, we can write for example

$$\psi_a(\vec r_i)\chi_{+,i} .$$

a) How many distinct two-particle product states can be constructed for identical particles 1 and 2 that are consistent with the Pauli exclusion principle? There is no distinction between which factor state you give to which particle: i.e.,

$$\psi_a(\vec r_1)\chi_{+,1}\psi_a(\vec r_2)\chi_{-,1} \qquad \text{and} \qquad \psi_a(\vec r_2)\chi_{+,2}\psi_a(\vec r_1)\chi_{-,2}$$

are the same product state for identical particles. Write down the product states. Are the product states orthornormal? If the particles were distinct, how many distinct two-particle product states could be constructed? How many distinct linearly-independent symmetrized states can be constructed from the two-particle product states? **HINT:** The first part is a problem of choosing k objects from n objects with no replacement and no distinction on ordering of choices.

b) Are the linearly-independent symmetrized states created from orthonormal product states of single particles always orthonormal? Prove your answer. **HINT:** The proof takes a bit of thinking.

c) Using the Slater determinant formalism construct from the part (a) product states all the symmetrized states in which the only one kind of single-particle spatial state occurs. Remember to normalize the symmetrized states. What kind of states are these in spin description?

d) Using the Slater determinant formalism construct from the part (a) product states all the symmetrized states in which two distinct single-particle spatial states occur. Remember to normalize the symmetrized states. What kind of states are these in spin description?

e) Two of the states constructed in the part (d) answer are neither triplet nor singlet states. But you can construct by linear combination a triplet state and singlet state from these two. Do so. Then you have full triplet-singlet set of symmetrized states comprising the two unused states from the part (d) answer and the two newly constructed states.

f) Discuss when you would expect the four symmetrizied states of the part (d) answer to be stationary states and when the you would expect the triplet-singlet set of symmetrized states to the stationary states.

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019 qfull 02200 3 5 0 tough thinking: 2-particle infinite square well

Extra keywords: (Gr-182:5.4)

6. The set of individual eigen states for a 1-dimensional, infinite square well confined to $[0, a]$ can be written $|n\rangle$ where $n = 1, 2, 3, \ldots$ The energies of the states are given by

$$E(n) = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 n^2$$

(e.g., Gr-26). For convenience $E_{\text{red}}(n) = n^2$ can be called the reduced energy of state n.

a) Say we have two non-interacting particles a and b in the well. Write write down the Hamiltonian for this case. The particles have the same mass m, but are not necessarily identical.

b) The reduced energy of a 2-particle state that satisfy the Schrödinger equation of part (a) can be written

$$E_{\text{red}}(n_1, n_2) = n_1^2 + n_2^2 \ .$$

Write a small computer code to exhaustively calculate the possible reduced energy levels up to and including $E_{\text{red}} = 50$ and the n_1 and n_2 combinations that yield these energies. The code should also calculate the degeneracy of each energy for the cases of non-identical particles, bosons, and fermions. I'll left you off easily, accidental degeneracies can be idendified by eye. (Note: An accidental degeneracy is when a distinct pair of n values (i.e., a pair not counting order) gives the same reduced energy.)

c) Write down the normalized vector expressions for all the 2-particle states up to the 4th allowed energy level for the cases of non-identical particles, identical bosons, and identical fermions. Just to get you started the non-identical particle ground state is

$$|a1, b1\rangle = |a1\rangle|b1\rangle \qquad \text{with} \qquad E_{\text{red}} = 2 \ .$$

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019 qfull 02300 3 5 0 tough thinking: exchange force

Extra keywords: (Gr-182)

7. Say we have orthonormal single-particle states $|a\rangle$ and $|b\rangle$. If we have distinct particles 1 and 2 in, respectively, $|a\rangle$ and $|b\rangle$, the net state is

$$|a1, b2\rangle = |a1\rangle|b2\rangle \ .$$

Of course, each of particles 1 and 2 could be in linear combinations of the two states if the states physically allowed the distinct particles to be in either one. In that case the linear combined state would be a four term state. But we have no interest in pursuing that digression at the moment.

Now two identical particles in states $|a\rangle$ and $|b\rangle$ have no choice, but to be in a symmetrized state by the symmetry postulate:

$$|1,2\rangle = \frac{1}{\sqrt{2(1+\delta_{ab})}}\left(|a1,b2\rangle \pm |a2,b1\rangle\right) ,$$

where the upper case is for identical bosons and the lower case for identical fermions. If the two states are actually the same state $|a\rangle$, then the state for bosons reduces to

$$|1,2\rangle = |a1,a2\rangle$$

and for fermions the state reduces to the null state $|0\rangle$ which is not a physical state, and thus the Pauli exclusion principle is incorporated in the state expression.

Note products of kets are actually tensor products (CT-154). In taking scalar products, the bras with index i (e.g., 1 or 2 above) act on the kets of index i. For example, for the state $|1a,2b\rangle = |a1\rangle|a2\rangle$ the norm squared is

$$\langle a1,b2|a1,b2\rangle = \langle a1|a1\rangle\langle a2|a2\rangle .$$

The fact that identical particles must be in symmetrized states means that their wave functions will be more or less clumped depending on whether they are bosons or fermions than if they could be fitted into simple product states like distinct particles. We are not bothering with the complication of spin for this problem. We will assume that all the particles are in the same spin state: e.g., they are all in the spin up state.

The clumping/declumping effect is called the **EXCHANGE FORCE**. Obviously, it is not really a force, but rather a result of the symmetrization principle requirements on physical states for identical particles. Still for some practical purposes one can certainly consider it as force. In this problem, we investigate the effect of the **EXCHANGE FORCE**.

a) Expand $\langle \Delta x^2\rangle = \langle (x_1 - x_2)^2\rangle$ into three terms that can be evaluated individually.

b) For the given two-particle state for **DISTINCT PARTICLES** $|a1,b2\rangle = |a1\rangle|b2\rangle$, formally show that

$$\langle \Delta x^2\rangle = \langle x^2\rangle_a + \langle x^2\rangle_b - 2\langle x\rangle_a\langle x\rangle_b ,$$

where the particle labels can be dropped from the single-particle state expectation values, but these values must be identified by the single-particle state that they are for: i.e., for states $|a\rangle$ and $|b\rangle$. What happens in the case that $|a\rangle = |b\rangle$? **HINT:** Remember that variance is defined by

$$\sigma^2 = \langle x^2\rangle - \langle x\rangle^2 .$$

c) There is an identity that is needed for part (d) and is useful in many other contexts. Say $|\alpha\rangle$ and $|\beta\rangle$ are general states (e.g., they could be one-particle or two-particle states). Say that

$$|\Psi\rangle = c_\alpha|\alpha\rangle + c_\beta|\beta\rangle$$

and we have general observable Q. We have the identity

$$\langle\Psi|\Psi\rangle = |c_\alpha|^2\langle\alpha|\alpha\rangle + |c_\beta|^2\langle\beta|\beta\rangle + 2\text{Re}(c_\alpha^* c_\beta\langle\alpha|Q|\beta\rangle) .$$

Prove the identity.

d) For the given two-particle state for **IDENTICAL PARTICLES**

$$|1,2\rangle = \frac{1}{\sqrt{2(1+\delta_{ab})}}\left(|a1,b2\rangle \pm |a2,b1\rangle\right) ,$$

determine $\langle \Delta x^2 \rangle$ for identical bosons and fermions. What happens in the case that $|a\rangle = |b\rangle$? **HINT:** Recall that

$$\langle a|b\rangle = \delta_{ab} \ ,$$

since the states are orthonormal.

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019 qfull 02400 2 5 0 moderate thinking: exchange force and infsq well

Extra keywords: (Gr-185:5.5) and the infinite square well

8. Imagine two non-interacting particles in an infinite square in the range $[0,a]$. Recall the eigenfunctions for this case are

$$\psi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$$

for $n = 1, 2, 3, \ldots$. Recall also the results of the Gr-182 and Gr-29:2.5 questions.

a) Say the particles are distinguishable and are in states n and m. What is $\langle \Delta x^2 \rangle = \langle (x_1 - x_2)^2 \rangle$ for this case? What is it if $n = m$?

b) Say the particles are identical bosons/fermions and are in the only allowed combination of states n and m. What is $\langle \Delta x^2 \rangle = \langle (x_1 - x_2)^2 \rangle$ for this case? What is it if $n = m$?

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019 qfull 02500 2 3 0 mod math: coupled simple harmonic oscillator, coupled SHOs

Extra keywords: On tests going to part f might be sufficient

9. There are two particles subject to separate simple harmonic oscillator (SHO) potentials. Initially, we assume that they are distinct particles. They are also coupled by a mutual SHO potential. The full Hamiltonian is:

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{1}{2}m_1\omega^2 x_1^2 + \frac{1}{2}m_2\omega^2 x_2^2 + \frac{1}{2}k(x_1 - x_2)^2 \ ,$$

where $k > 0$ which in this context means the interaction is attractive. The problem is 1-dimensional: it is in the x dimension only.

a) Write down the formulae for the center-of-mass (CM) and relative (REL) coordinate and their inverses (i.e., x_1 and x_2 expressed in terms of the CM coordinate X and the relative x).

b) Transform the Hamiltonian to the center-of-mass-relative (CM-REL) coordinates (showing all the steps).

c) Now show that the time-independent Schrödinger equation for the Hamiltonian separates into CM and REL time-independent Schrödinger equations. Define

$$\tilde{\omega} = \sqrt{\omega^2 + \frac{k}{\mu}} = \omega\sqrt{1 + \frac{k}{\mu\omega^2}}$$

(where μ is the reduced mass) in order to simplify the REL equation. Does the overall time-independent Schrödinger equation have an exact solution?

d) Write down the general expression for the eigen-energies of the total stationary states in terms of the SHO quantum numbers $n_{\rm CM}$ and $n_{\rm REL}$ for the respective CM and REL parts.

e) Next write the expression for the eigen-energies in the case that $k = 0$. Define a new quantum number n that alone gives the eigen-energy and the degeneracy of the eigen-energy. What is the degeneracy of an eigen-energy of quantum number n?

f) Now assume that $k > 0$, but that $k/(\mu\omega^2) << 1$. Write down a 1st order correct expression for the energy in terms of n and $n_{\rm REL}$. Give a schematic energy-level diagram.

g) Now assume that $k/(\mu\omega^2) >> 1$. Give a schematic energy-level diagram in this case.

h) Now assume that the two particles are identical spin-0 bosons. Note that identical means they now have the same mass. Given the symmetry requirement for boson states, which solutions (specified by the $n_{\rm CM}$ and $n_{\rm REL}$ quantum numbers) are not physically allowed?

i) Now assume that the two particles are identical spin-1/2 fermions. Note again that identical means they now have the same mass. But also note they arn't electrons. Their interactions are determined by the given Hamiltonian only. Because the particles are spin-1/2 fermions, the stationary state wave functions for system must be multiplied by appropriate eigenspinors to specify the full stationary state. Given the antisymmetry requirement for fermion states, what restrictions are put on the wave function and spinor quantum numbers of an eigenstate?

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019 qfull 02600 1 5 0 easy thinking: symmetrization, Slater determinant
Extra keywords: (Gr-187:5.7)

10. Say that you solve a Schrödinger equation for N identical particles to get the normalized wave function $\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \ldots, \vec{r}_N)$. How would you symmetrize the wave function for bosons? Then how would you symmetrize for fermions all in the spin-up state so that you don't have spinors to complicate the question? How would you normalize the wave function?

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019 qfull 02700 1 5 0 easy thinking: doubly excite He decay
Extra keywords: (Gr188.58a)

11. Say you put two electrons into the $n = 2$ principle quantum number shell of a neutral helium atom and immediately one electron is ejected and the other decays to the ground of the He$^+$ ion. What approximately is the kinetic energy of the ejected electron. **NOTE:** Without a detailed specification of the doubly-excited helium atom we cannot know exactly what the energies of the excited electrons are. There are two simple approximate choices for their energies: 1) assume that the energy levels of the singly-excited helium atom apply (see, e.g., Gr-189); 2) assume that the $Z = 2$ hydrogenic energy levels apply. The first choice is probably most in error because it assumes too much electron-electron interaction: the electrons may further apart in the actual doubly-excited state; but, in fact, where they are depends on exactly what doubly excited state they are in. The 2nd choice is certainly wrong by assuming zero electron-electron interaction.

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019 qfull 02900 2 5 0 moderate thinking: helium with bosons
Extra keywords: (Gr-188:5.9)

12. Describe qualitatively how the helium atom energy level diagram would plausibly change under the following conditions.

a) Say the electrons were spin zero bosons.

b) Say the electrons were spin 1/2 bosons—a contradiction in postulates, but for the sake of argument have it so.

c) Say the electrons were spin 1/2 fermions, but were quantum mechanically distinguishable particles. **HINT:** In this case the answer is going to be pretty much indefinite.

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019 qfull 03000 2 5 0 moderate thinking: Bose-Einstein counting
Extra keywords: See Po-13 and Po-47

13. In statistical mechanics, the symmetrization requirement on identical bosons enters in the way that probabilities are assigned to the global states they can form. We will investigate how symmetrization manifests itself in this case.

a) Say you had g single-particle states and n distinct particles. How many distinct global states can you form? What is the probability of each global state assuming that each has equal probability?

b) Now a trickier case. Say you had g single-particle states and n identical particles. The probability p_i that a particle goes into single-particle state i is **INDEPENDENT** of what the other particles do: note $\sum_{i=1}^{g} p_i = 1$, of course. You can construct all possible global states by inserting one particle at a time into the system—can you imagine a global state that cannot be so constructed? Say you do insert the n particles one at a time to the system. The probability of an n-particle global state formed by the insertion sequence $ijk\ldots\ell$ is $p_i p_j p_k \ldots p_\ell$ which has n factors, of course. But because the particles are identical, each (distinct) global state can be constructed in general by multiple insertion sequences. How many distinct insertion sequences for n particles correspond to a single global state with occupation number set $\{n_i\}$? If all the p_i are equal, what is the probability of a global state with occupation number set $\{n_i\}$ formed by random insertion of particles?

The sum of the probabilities for all insertion sequences is 1. Why must this be so on general grounds? Now prove more explicitly that the sum of all inserttion sequence probabilities is 1. **HINT:** Consider

$$1 = \left(\sum_{i=1}^{g} p_i \right)^n$$

and a proof by induction.

c) Now in the part (b) answer, we didn't find out how many distinct global states there were. To find this out you need a different counting procedure. Let's consider finding all possible global states given the following conditions. Imagine that all n particles were distinct and that the order in which you choose the single-particle states to slot them into also matters. To start with you must select a state: you can't put a particle in a non-state. Then proceed selecting a particle for the current state or a new state until you are out of particles and states. Now did the order of the states matter or the order of the choice of particles?

d) Now for classical, non-interacting particles randomly slotted into single-particle states, the probability of each global state is as determined in part (b). Quantum mechanical non-interacting bosons do not act like classical particles. Because of the symmetrization principle—in a way the instructor has never found out—each distinct global state has equal probability. What is this probability for n bosons in g single-particle states? Say that we have all n bosons in one single-particle state. What is the classical probability of this global state? Which is larger the classical probability or the boson probability? What does the last result suggest about the random distributions of bosons relative to classical random distributions?

e) Consider two identical coins—say quarters. How many distinct global physical states can be made given that the single-coin states are head and tail? Now toss them up together in a completely randomizing way 36 times. Count the number of distinct global states of each kind that you get? Do the probabilities of each distinct global state appear to be classically random or boson random?

Chapt. 20 Atoms

Multiple-Choice Problems

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020 qmult 00100 1 1 1 easy memory: atom defined

1. An atom is a stable bound system of electrons and:

   a) a single nucleus. b) two nuclei. c) three nuclei. d) a single quark.
   e) two quarks.

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020 qmult 01000 1 4 1 easy deducto-memory: central potential

2. "Let's play *Jeopardy*! For \$100, the answer is: A favored approximation in the simpler solutions for the electronic structure of atoms in quantum mechanics."

   What is the ____________, Alex?

   a) central potential approximation b) non-central potential approximation
   c) grand central approximation d) atom-approximated-as-molecule method
   e) electrons-as-bosons approximation

Full-Answer Problems

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020 qfull 00200 1 3 0 easy math: electronic configurations to Ca

1. Write down the ground state electronic configurations of the neutral atoms from hydrogen (element 1) to calcium (element 20). Write down the element symbols too.

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020 qfull 00400 1 5 0 easy thinking: spectrum of He II

Extra keywords: (Gr-188:58b)

2. Describe the spectrum of He II (i.e., singly-ionized helium or He^+) sans perturbations..

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020 qfull 00410 3 3 0 tough math: helium atom 1st order perturbation

Extra keywords: (Gr-188:5.10)

3. If one neglects the electron-electron interaction of the helium atom then the spatial ground state is just the product of two hydrogenic states:

$$\psi(\vec{r}_1,\vec{r}_2)=\psi_{100}(\vec{r}_1)\psi_{100}(\vec{r}_2)=\frac{1}{\pi a_{\mathrm{He}}^3/8}e^{-2(r_1+r_2)/a}=\frac{8}{\pi a^3}e^{-2(r_1+r_2)/a} ,$$

where $a_{\mathrm{He}}=a/Z=a/2$ is the helium Bohr radius and a is the standard Bohr radius (see, e.g., Gr-137–138 and Gr-187). The 1st order perturbation correction to the helium atom ground state is given by

$$\langle H'\rangle ,$$

where H' is the perturbation Hamiltonian: i.e.,

$$\frac{e^2}{4\pi\epsilon_0}\frac{1}{|\vec{r}_1-\vec{r}_2|}$$

in MKS units (see, e.g., Gr-187) or

$$\frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$$

in Gaussian CGS units. Note that we use e for both fundamental charge unit and the exponential factor: this is conventional of course: context must decide which is which.

a) Analytically calculate

$$\left\langle \frac{1}{|\vec{r}_1 - \vec{r}_2|} \right\rangle .$$

HINTS: Set

$$|\vec{r}_1 - \vec{r}_2| = \sqrt{r_1^2 + r_2^2 - 2r_1r_2\mu} ,$$

where $\mu = \cos\theta$ is the angle cosine between the vectors. Integrate over all $\vec{r}_2$ space first taking $\vec{r}_1$ as the z axis for spherical coordinates. It helps to switch to dimensionaless variables earlier on. There are no specially difficulties or tricks: just a moderate number of steps that have to be done with tedious care.

b) Now the expression for a hydrogenic energy level, sans perturbations, is

$$E_n = -\frac{1}{2}m_e c^2\alpha^2\frac{Z^2}{n^2} = -\frac{Z^2E_{\text{ryd}}}{n^2} \approx -\frac{13.6Z^2}{n^2}\ \text{eV} ,$$

where m_e is the electron mass, α is the fine structure constant, Z is the nuclear charge, and $E_{\text{ryd}} \approx 13.6\,\text{eV}$ is the Rydberg energy (see, e.g., Ga-197). In Gaussian CGS units

$$\alpha = \frac{e^2}{\hbar c} \qquad \text{and} \qquad a = \frac{\hbar}{m_e c\alpha}$$

(e.g., Ga-199). What is the energy of the helium atom ground state in terms of Rydberg energies and eVs?

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020 qfull 01000 2 5 0 moderate thinking: quantum defects

Extra keywords: (MEL-220:9.1) Needs some more work, particularly (b)

4. Excited states of atoms can usually be approximated as merely promoting a valence electron to a single-particle state at a higher energy than any of the ones used in the ground state. For high energy single-particle states one often finds that their energies form a quasi-Rydberg series: i.e.,

$$E_{n\ell} \approx -\frac{E_{\text{Ryd}}}{(n-\mu_{n\ell})^2} ,$$

where n is the principal quantum number, ℓ is the angular momentum quantum number, $E_{\text{Ryd}} = 13.606\,\text{eV}$ is the Rydberg energy, and $\mu_{n\ell}$ is the quantum defect. I suppose quantum defect gets its name since it accounts for a "defect" in the quantum number. When quantum defects are small the wave functions will be quasi-hydrogen-like and hydrogen-like approximations can be used with some confidence—which is often an immense simplification. (Note I use hydrogen-like, not hydrogenic: hydrogen-like implies that the central potential is like e^2/r, whereas hydrogenic implies the central potential is like $Z_{\text{N}}e^2/r$—at least that's the way it is in this question. Various uses can be made of the quantum defect parameterization of energy (e.g., Mi-97).

In understanding quantum defects, three facts are useful to know. First, the single-particle potential well outside of the core approximates

$$V(r) = -\frac{e^2}{r}$$

for a neutral atom. Second, near the nucleus of the atom, the single-particle potential approximates the bare nucleus potential

$$V(r) = -\frac{Z_{\mathrm{N}}e^2}{r} ,$$

where Z_{N} is the nuclear charge. Third, wave functions in central potentials for small radius tend to go as r^ℓ. This result is rather robust since it is true of hydrogenic wave functions (MEL-57; Ar-622) and spherical Bessel functions (Ha-37) which are the radial solutions of the infinite spherical well. Only s states (i.e., $\ell = 0$ states) have non-zero probability amplitude at $r = 0$.

a) Find the formula for the quantum defect in terms of the energy of the energy level. Then compute the quantum defects for sodium and lithium given the following table. **HINT:** A computer program would lessen the labor.

Table: Observed Energy Levels in Electronvolts (not to modern accuracy)

	n	s	p	d	f
Li					
	2	−5.3923	−3.5442	...	...
	3	−2.0188	−1.5577	−1.5133	...
	4	−1.0509	−0.8701	−0.8511	−0.8502
	5	−0.6432	−0.5544	−0.5446	−0.5434
Na					
	3	−5.1397	−3.0359	−1.5223	...
	4	−1.9480	−1.3863	−0.8557	−0.8507
	5	−1.0229	−0.7946	−0.5472	−0.5445
	6	−0.6297	−0.5150	−0.3797	−0.3772

b) As you can see from your table of quantum defects, the quantum defects are **NOT** nearly zero in general as they would be if the states were almost exactly hydrogen-like at their principal quantum number. Also the quantum defects are **NOT** just equal to the principal quantum number of highest core shell n_{core}: i.e., they are not 1 for Li and 2 for Na. Thus, the quantum defect shows that the outer states are not hydrogen-like either for their actual principal quantum number n nor at an effective principal quantum number $n - n_{\mathrm{core}}$. Why are these two a priori guesses for quantum defects wrong even though the potential is close to that of hydrogen with $Z_{\mathrm{N}} = 1$ in the region where the bulk of the probability for outer states is located.

c) Give a reason why quantum defects should have positive values if they are significantly large. Why might small quantum defects be negative?

d) Why do quantum defects decrease with ℓ?

e) Explain why the Na quantum defects tend to be larger than the Li quantum defects?

f) Give a reason why quantum defects may not vanish as $n \to \infty$.

Chapt. 21 Molecules

Multiple-Choice Problems

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021 qmult 00100 1 1 1 easy memory: molecule defined

1. A stable bound system of electrons and more than one nucleus with some specific recipe for the numbers of each kind of nuclei is:

   a) a molecule.
   b) an atom.
   c) a nucleon.
   d) a fullerene.
   e) a baryon.

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021 qmult 00100 1 4 1 easy deducto-memory: atoms bound in molecules

2. "Let's play *Jeopardy*! For \$100, the answer is: Because they are formed by bonding atoms and dissociate into atoms?"

   a) What is one good reason for thinking of molecules as bound atoms, Alex?
   b) What are three bad reasons for thinking of molecules as bound atoms, Alex?
   c) What is no reason at all for thinking of molecules as bound atoms?
   d) What is ambiguous answer, Alex?
   e) What is am-Piguous answer, Alex?

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021 qmult 00300 2 1 2 easy memory: molecular energy scales

3. Given electron mass m and typical nuclei mass M, the ratio of electronic, vibrational, and rotational energies for a molecule is of order:

   a) $1 : 1 : 1$.
   b) $1 : (m/M)^{1/2} : (m/M)$.
   c) $1 : (m/M) : (m/M)$.
   d) $1 : (m/M)^{1/4} : (m/M)^{1/2}$.
   e) $1 : (m/M)^{1/4} : (m/M)^{1/3}$.

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021 qmult 00400 1 4 4 easy deducto-memory: Born-Oppenheimer approx.
Extra keywords: (Ba-473)

4. "Let's play *Jeopardy*! For \$100, the answer is: This approximation allows one to treat the nuclei in atoms as though they interacted only with an effective potential constructed from actual potentials and the electronic kinetic energy (i.e., the total electronic energy)."

   a) What is the Alpher-Behte-Gamow recipe, Alex?
   b) What is the Einstein-Woody-Allen approximation, Alex?
   c) What is the linear combination of atomic orbitals method, Alex?
   d) What is the Born-Oppenheimer approximation, Alex?
   e) What is the tight-binding approximation, Alex?

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021 qmult 00500 1 4 5 easy deducto-memory: tight-binding theory

5. "Let's play *Jeopardy*! For \$100, the answer is: It posits that overlapping wave functions of bound atoms can be treated to some degree in terms of the orbitals of isolated atoms."

   a) What is the genetic algorithm method, Alex?
   b) What is the linear variational method, Alex?
   c) What is tight-binder theory, Alex?
   d) What is tight-wadding theory, Alex?
   e) What is tight-binding theory, Alex?

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021 qmult 00600 1 1 3 easy memory: LCAO

6. In LCAO (linear combinations of atomic orbitals method) one uses atomic orbitals as a non-orthonormalized basis set for constructing:

   a) bound states of nucleons.
   b) bound states of photons.
   c) inter-atomic bonding and anti-bonding states.
   d) intra-atomic stationary states.
   e) property-law violating beach-front homes in California.

Full-Answer Problems

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021 qfull 00100 2 5 0 moderate thinking: universal sp-coupling parameters

Extra keywords: See Ha-95

1. Harrison (Ha-95) presents "universal" sp-bond matrix elements or coupling pararameters:

$$\langle \mathrm{s}_1|H|\mathrm{s}_2\rangle = V_{\mathrm{ss}\sigma} = -\frac{\pi^2}{8}\frac{\hbar^2}{md^2} \ ,$$

$$\langle \mathrm{p}_{z1}|H|\mathrm{p}_{z2}\rangle = V_{\mathrm{pp}\sigma} = \frac{3\pi^2}{8}\frac{\hbar^2}{md^2} \ ,$$

$$\langle \mathrm{s}_1|H|\mathrm{p}_{z2}\rangle = V_{\mathrm{sp}\sigma} = \frac{\pi}{2}\frac{\hbar^2}{md^2} \ ,$$

and

$$\langle \mathrm{p}_{x1}|H|\mathrm{p}_{x2}\rangle = \langle \mathrm{p}_{y1}|H|\mathrm{p}_{y2}\rangle = V_{\mathrm{pp}\pi} = -\frac{\pi^2}{8}\frac{\hbar^2}{md^2} = V_{\mathrm{ss}\sigma} \ ,$$

where 1 and 2 denote two atoms aligned along the z-axis, H is the single-particle Hamiltonian owing to the cores of the two atoms, the $|s_1\rangle$, etc., are single-particle atomic orbitals (radial parts of some sort times the cubical harmonics for the angular parts) oriented relative to a common set of axes, d is the inter-nuclei separation, and $V_{\mathrm{sp}\sigma}$ has a π, not π^2. The s and p subscripts on the V's indicate the atomic orbitals in the coupling and the σ and π indicate the indicates the quantum numbers m^2 of L_z^2 operator of the molecular orbitals that result from the coupling of the different states: σ is for $m^2 = 0$ and π is for $m^2 = 1$.

The reason for the complication of using the eigenvalues of the L_z^2 operator rather than the L_z operator is that the $|\mathrm{p}_x\rangle$ and $|\mathrm{p}_y\rangle$ cubical harmonics are eigenstates of L_z^2, but not of L_z. Recall the lowest quantum number spherical harmonics $Y_{\ell,m}$ are

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}} \ , \qquad Y_{1,0} = \sqrt{\frac{3}{4\pi}}\cos(\theta) \ , \qquad \text{and} \qquad Y_{1,\pm 1} = \sqrt{\frac{3}{8\pi}}\sin(\theta)e^{\pm im\phi} \ ,$$

where ℓ is the L^2 quantum number, m is the L_z quantum number, θ is the angle from the z-axis, and ϕ is the azimuthal angle. The cubical harmonics are defined by

$$|\mathrm{s}\rangle = Y_{0,0} = \frac{1}{\sqrt{4\pi}} \ ,$$
$$|\mathrm{p}_x\rangle = \frac{Y_{1,1}+Y_{1,-1}}{\sqrt{2}} = \sqrt{\frac{3}{4\pi}}\frac{x}{r} \ ,$$
$$|\mathrm{p}_y\rangle = \frac{Y_{1,1}-Y_{1,-1}}{i\sqrt{2}} = \sqrt{\frac{3}{4\pi}}\frac{y}{r} \ ,$$

and

$$|\mathrm{p}_z\rangle = Y_{1,0} = \sqrt{\frac{3}{4\pi}}\frac{z}{r} \ .$$

a) Verify that polar plots of the "p" cubical harmonics are a touching pair of spheres of radius $\sqrt{3/(4\pi)}/2$. (I mean, of course, when you consider the plots as spherical polar coordinate plots.) For $|\mathrm{p}_z\rangle$, for example, the spheres touch at the z-axis origin and are aligned with the z-axis: the upper sphere is "positive" and the lower sphere is "negative": i.e., the radial position from the origin comes out a negative number: one just plots the magnitude. **HINTS:** It is sufficient to do the proof for $|\mathrm{p}_z\rangle$, since the others are the same *mutatis mutandis.* A diagram would help.

b) Interpret the physical significance of the polar plots of the cubical harmonics.

c) Show that $|\mathrm{p}_x\rangle$ and $|\mathrm{p}_y\rangle$ are eigenstates of L_z^2, but not L_z. What other angular momentum operators are they eigenstates of? **HINT:** Recall

$$L_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi} \ .$$

d) Now we come to the question yours truly wanted to ask before chronic digression set in. Write sp-bond coupling parameters in terms of fiducial values in units eV-Å^2: e.g.,

$$\frac{C}{d_{\text{Å}}^2} \ ,$$

where C is a numerical constant (i.e., an actual value) in eV-Å^2 and $d_{\text{Å}}$ is mean nuclei separation in Angstroms. Then evaluate the constants for $d_{\text{Å}} = 3$. **HINT:** Recall

$$\frac{\hbar^2}{m} = 7.62\,\text{eV-Å}^2 \ ,$$

where m is the electron mass.

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021 qfull 00300 2 3 0 easy math: Li2 with spin

Extra keywords: Reference Ha-72

2. Let us consider the single-particle bonding and antibonding states and their energies for Li_2. We assume that the single-particle Hamiltonian of the Li_2 molecule is

$$H = \frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r}) = \frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r}-\vec{r}_1) + V(\vec{r}-\vec{r}_2) \ .$$

where $\vec{r}$ is measured from the midpoint between the nuclei, $\vec{r}_1$ is the position of nucleus 1, and $\vec{r}_2$ the position of nucleus 2. We are assuming the nuclei are at fixed positions which is the crudest Born-Oppenheimer approximation. The observed equilibrium separation of the nuclei is $d = 2.67\,\text{Å}$: we take this to be the fixed separation. We will make the LCAO (linear combination of atomic orbitals) approximation.

a) Use the linear variational method to calculate the the bonding and antibonding states and their energies. The basis states are the two atomic orbital 2s states of the atoms: call them $|1\rangle$ and $|2\rangle$. We assume $|1\rangle$ and $|2\rangle$ are knowns: they have the same energy $\varepsilon_{\rm s} = -5.34\,\text{eV}$. Assume the basis states are orthogonal: a poor approximation actually, but this problem is intended to be heuristic. Make a reasonable approximation to evaluate the diagonal matrix elements. For off-diagonal or coupling matrix elements use

$$V_{\rm ss\sigma} = -\frac{\pi^2}{8}\frac{\hbar^2}{md^2} = -\frac{9.40\,\text{eV-Å}}{d_{\text{Å}}^2} \ .$$

this is one of Harrison's "universal" sp-bond couplings (Ha-95). Which state is the bonding state and which the antibonding state and why are they so called?

b) What is the component of orbital angular momentum of single-particle states about the inter-nuclear axis? How do you know this? What symbol represents this orbital angular momentum component value for molecules? **HINT:** Recall that the z-component orbital angular momentum operator is

$$L_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi} \ ,$$

where ϕ is the azimuthal angle about the z-axis (MEL-23).

c) Now construct six plausible symmetrized two-particle states including spinor from our bonding and antibonding position states: a ground state and the five excited states. So everyone is on the same wavelength let

$$\alpha = \begin{pmatrix}1\\0\end{pmatrix} \qquad \text{and} \qquad \beta = \begin{pmatrix}0\\1\end{pmatrix} \ .$$

What are the approximate energies of these states? Can we construct any more states from the bonding and antibonding states? We, of course, are assuming that there is no spin operator in the Hamiltonian. **NOTE:** These states may not be very realistic: this is just an exercise.

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021 qfull 03000 2 5 0 moderate thinking: molecular relative coordinates

Extra keywords: A misconcieved problem.

3. One usually wishes to separate the center of mass and relative parts of the nuclei part of a molecular wave function. For two nuclei, the situation is a two-body problem and can be treated like hydrogenic systems (Da-334). For the general multiple nuclei case, a different approach is needed that treats all nuclei on the same footing. Let $\vec{r}_i$ be nucleus i's position relative to an external inertial frame. Let $\vec{r}_i'$ be nucleus i's position relative to $\vec{R}$ the molecular center of mass. We make the approximation that the electrons can be neglected in evaluating the center of mass. **NOTE:** I was fooled into thinking there was neat way of doing this. The cross term doesn't vanish. But one probably has to construct independent coordinates in a special way for each kind of molecule. But maybe something is salvageable so I'll leave this around for now.

a) Express $\vec{R}$ and $\vec{r}_i'$ in terms of the positions $\vec{r}_i$.

b) Now express the operators $\partial/\partial x_i$ and $\partial^2/\partial x_i^2$ in terms of operators $\partial/\partial x_i'$ and $\partial/\partial X$. For simplicity we only consider the x-components of the various coordinates. The y- and z-components are handled similarly.

c) Now show that

$$H = \sum_i \frac{p_i^2}{2M_i} + V(\{r_i\}) = \frac{p_{\rm cm}^2}{2M_{\rm tot}} + \sum_i \frac{p_i'^2}{2M_i'} + V(\{r_i'\}) \ ,$$

where H is the Hamiltonian of the nuclei in the effective potential $V(\{r_i\})$ (the curly brackets mean “set of”) with no external potential present, p_i' are the relative coordinate momentum operators, and

$$M_i' = \frac{M_i}{[1-(M_i/M_{\rm tot})]^2} \ .$$

Chapt. 22 Solids

Multiple-Choice Problems

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022 qmult 00100 1 1 3 easy memory: simplest quantum mechanical solid model

1. The simplest quantum mechanical solid model is arguably:

   a) the hydrogen atom. b) the helium atom. c) the free electron gas model.
   d) the infinite periodic potential model. e) the finite periodic potential model.

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022 qmult 00110 1 1 1 easy memory: infinite square boundary conditions

2. For the simple free electron gas model of a solid, one choice of boundary conditions out of two possibilities is ____________ boundary conditions.

   a) infinite square well b) finite square well c) Gaussian well d) hydrogen atom
   e) helium atom

---

022 qmult 00130 1 4 4 easy deducto-memory: periodic boundary conditions
Extra keywords: mathematical physics

3. "Let's play *Jeopardy*! For $100, the answer is: These quantum mechanical boundary conditions for solids, also known a Born-von-Karman boundary conditions, are not realistic in most cases. They are realistic in some cases. For example, for the dimension of a solid that forms a closed loop: e.g., a solid that has donut shape can be have an angular coordinate that must be periodic by symmetry over the range $[0°, 360°]$. But whether realistic or not, it can be shown that they lead to the same average behavior as realistic boundary conditions for macroscopically large solid samples.

   Why are these boundary conditions used at all? Well for one thing they are an ideal kind of boundary conditions that are completely independent of what the surface behavior of solid is. Thus, they are neutral case. For another thing they are easy to use in developments in particular when dealing with periodic potentials in a solid."

   What are ____________ boundary conditions, Alex?

   a) infinite square well b) aperiodic c) Rabi-Schwinger-Baym-Sutherland
   d) periodic e) relaxed

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022 qmult 00500 1 4 5 easy deducto-memory: Bloch's theorem
Extra keywords: mathematical physics

4. "Let's play *Jeopardy*! For $100, the answer is: It is a theorem in quantum mechanics that applies to systems with periodic potentials. In one dimension, say one has the periodic potential

$$V(x) = V(x + a)$$

where a is the period distance The theorem then says that the wave function must satisfy

$$\psi(x + a) = e^{Ka}\psi(x) \qquad \text{or} \qquad \psi(x) = e^{Ka}\psi(x - a)$$

or

$$\psi(x + na) = e^{Kna}\psi(x) \qquad \text{or} \qquad \psi(x) = e^{Kna}\psi(x - na) \ ,$$

where K is wave number quantity and n is any integer. Say that one has $\psi(x)$ for the range $[0, a]$. Then the $\psi(x)$ for the range $[na, (n+1)a]$ can be evaluated from the last formula: e.g.,

$$\psi(na) = e^{Kna}\psi(0) \qquad \text{and} \qquad \psi[n+1)a] = e^{Kna}\psi(a) \text{ .''}$$

What is ____________, Alex?

a) Lorentz's theorem b) Einstein's rule c) Schrödinger's last theorem
d) Born's periodicity law e) Bloch's theorem

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022 qmult 00530 1 1 3 easy memory: Dirac comb

5. A periodic potential that consists a periodic array of equally strong Dirac delta function potential spikes separated by flat potential reigons is called a ____________ comb.

a) Bloch b) Compton c) Dirac d) Fermi e) Pauli

Full-Answer Problems

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022 qfull 00100 2 5 0 moderate thinking: free electron gas model of a solid

Extra keywords: (Ha-324:2.4)

1. The free electron gas model of a solid is arguably the simplest model of solid. The electrons are assumed to be non-interacting fermions confined to a potential well. The background of positive ions and the electrons's own Coulomb force combine to create the potential well. The potential inside the well is flat. The most obvious set of boundary conditions are infinite square well boundary conditions.

   Periodic boundary conditions (AKA Born-Von-Karman boundary conditions) are also used. They give the same macroscopic results as infinite square well boundary conditions and are better suited for treating periodic potentials inside solids. Periodic boundary conditions actually means you imagine space looping back on itself for opposing ends of a rectangular box. If you go out one end, you come back in the opposing end. If we assume a 1-dimensional wave function along a box dimension (which we actually require in our development in this problem), then we demand that that wave function be single-valued as it loops around and around through looped space. We have no physical meaning for a multi-valued wave function. You could at first imagine that there could be a discontinuity in the wave function as it crosses a boundary. But the ordinary continuity conditions on a wave function at locations of finite potential require that the wave function and its 1st derivative must be continuous across the boundary. Thus, to loop back into itself, the wave function and its 1st derivative must have the same values at opposing boundaries.

   Let us consider a free electron gas model of a solid in 1, 2, and 3 dimensions simultaneously. Use periodic boundary conditions in all three cases: a 1-dimensional rectangular box is a line segment, a 2-dimensional rectangular box is a rectangle, and a 3-dimensional rectangular box is what one ordinarily means by a rectangular box. Let L_i be the length of side i of the rectangular box and $V = \prod_i L_i$ be the rectangular box volume. Let ℓ be the number of dimensions.

   a) Solve the time-independent Schrödinger equation for the single-particle stationary states for all three dimension cases. These states can be called k states since they distinguished by their wavenumbers for the available dimensions. Normalize the solutions solutions and give their quantization rules for wavenumber and energy. **HINT:** You must separate the multi-particle time-independent Schrödinger equation.

   b) Each single-particle stationay k state can be located in what is called k-space by a wavenumber vector $\vec{k} = (k_1, k_2, k_2)$, where we have used 1, 2, and 3 to label the dimensions. What is the volume V_k in k-space of the k-space rectangular boxes that are centered on the stationary state wavenumber vector tips and tile all k-space without gaps or overlaps and are all of the same size. The volume V_k is the k-space volume per state. What is the average density of spatial states in k-space ρ_k?

c) We now make the continuum approximation which is valid for samples that are macroscopic in all available dimensions. This means that we treat the average density of spatial states in k-space as if it were an uniform density. Find the expression for the differential number of states dN_k per unit space volume in a spherical shell in k-space. The shell radius is k and its thickness is dk. Include the spin degeneracy by a factor g which equals 2 for spin 1/2 electrons. But leave g unevaluated. By leaving g unevaluated, one can track how the spin degeneracy affects dN_k and expressions derived from dN_k.

d) The Pauli exclusion principle for fermions requires that each single particle k state (where the states now thought of as distinguished by both wavenumber vector and spin state) have only one fermion at most. This statement must be qualified. What it really means is that the product wave function of single particle states can have each distinct single-particle state included once only. If there are N fermions, the overall symmetrized wave function contains $N!$ versions of the product wave function with the individual particle coordinate labels in all possible permuations. But we don't have to worry about product wave functions or symmetrized wave functions explicitly in the free electron gas model of solids. We simply make use of the Pauli exclusion principle to say that the single-particle states can only be used once in calculating results or to put this in common jargon only one electron can occupy at single particle state at most.

Now in the ground state of (which is the absolute zero temperature state) in our free electron gas model, the electrons occupy the lowest energy single-particle states consistent with the Pauli exclusion principle. This means in k-space, the electrons occupy a sphere of radius k_F where F where stands for Fermi. Since F stands for a name, not a variable it ought to be in Roman, not Italic, font, but convention seems to dictate Italic font (e.g., Gr-221, CT-1435). (I guess since Fermi was Italian ...) The radius k_F is called the Fermi wavenumber. The sphere is called the Fermi surface. It's not called the Fermi sphere usually since the concept of Fermi surface applies to periodic potential cases, where in general the Fermi surface is not a sphere.

Using the results of the part (c) answer solve for k_F in general and explicitly for the 3 dimensional cases. Assume the electron density (in space space) is $n_e = N/V$.

e) Now solve for the Fermi energy E_F in general and for the 3 dimensional cases.

f) What is ρ_E: i.e., the density of states per unit space volume per unit energy in the continuum of states approximation. Write a general formula that is valid for all three dimension cases. **HINT:** One requires the same number of states between any corresponding limits: i.e.,

$$dN = \rho_{k\ \mathrm{shell}}\, dk = \rho_E\, dE\ ,$$

where $\rho_{k\ \mathrm{shell}}$ is the density of k states in the differential k space shell dk. The general expression for $\rho_{k\ \mathrm{shell}}$ must have turned up in the part (c) answer without so labeling it.

g) Now solve for the total energy per unit space volume $\mathcal{E}$ of the ground state for electron density n_e. Also find E_{ave} the average energy of the electrons. Don't bother to expand E_F using the expressions from the part (e) answer. The formulae for this answer are long enough as it is. Just do the general dimensional case for $\mathcal{E}$, but show all the dimensional cases explicitly for E_{ave}.

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022 qfull 00110 1 3 0 easy math: free electron gas formulae and fiducial formulae

2. For a free electron gas (in 3 dimensions) at abolute zero temperature, the Fermi energy is given

by

$$E_F = \frac{\hbar^2}{2m}\left[\left(\frac{2}{g}\right)(3\pi^2)n_e\right]^{2/3} ,$$

where $\hbar$ is Planck constant divided by 2π, m is the electron mass, $g = 2$ is the spin 1/2 particle degeneracy, and

$$n_e = \frac{N}{V}$$

is the free electron density with N being the number of electrons and V being the sample volume. The average energy per electron E_{ave} is given by

$$E_{\text{ave}} = \frac{3}{5}E_F .$$

For this question, you will need the following constants,

$$\begin{aligned}
e &= 1.602176487(40)\times 10^{-19}\,\text{C} ,\\
m &= 9.10938215(45)\times 10^{-31}\,\text{kg} ,\\
mc^2 &= 510998.910\,\text{eV} ,\\
k_{\text{B}} &= 1.3806504(24)\times 10^{-23}\,\text{J/K} ,\\
\hbar &= 1.054571628(53)\times 10^{-34}\,\text{J, s} ,\\
m_{\text{amu}} &= 1.660538782(83)\times 10^{-27}\,\text{kg} .
\end{aligned}$$

a) Free electron density can be expressed in terms of ordinary density (AKA mass density) ρ by

$$n_e = \frac{\rho}{m_{\text{amu}}}\sum_i \frac{X_i Z_i}{A_i} ,$$

where the sum is over all atoms in the sample, X_i is the mass fraction of atom i, Z_i is the number of free electrons per atom for atom i, and A_i is the atomic weight of atom i. Convince yourself that this formula makes sense. Actually the formula can be simplified by introducing the mean mass per electron μ_e defined by

$$\frac{1}{\mu_e} = \sum_i \frac{X_i Z_i}{A_i} .$$

Take $1000\,\text{kg/m}^3$ as a fiducial value for ρ (which is just like writing density in grams per cubic centimeter). Take 50 as a fiducial value for μ_e: this is like an element in the atomic weight vicinity of iron with one valence electron delocalized. Now write n_e in terms of fiducial values: i.e., find the coefficient in the formula expression

$$n_e = \text{coefficient} \times \frac{\rho}{1000\,\text{kg/m}^3}\frac{50}{\mu_e} ,$$

The coefficient is a fiducial electron density.

b) Now find the formula for E_F in terms of fiducial values both for joules and electronvolts: i.e., find the coefficient in the formula

$$E_F = \text{coefficient} \times \left[\left(\frac{2}{g}\right)\frac{\rho}{1000\,\text{kg/m}^3}\frac{50}{\mu_e}\right]^{2/3} .$$

The coefficient is a fiducial Fermi energy. Are solids in human environments relativistic?

c) Now find the formula for the Fermi temperature $T_F = E_F/k_{\rm B}$ in terms of fiducial values both for joules and electronvolts. The coefficient is a fiducial Fermi temperature. Are solids in human environments hot or cold in comparison to the Fermi temperature?

d) Now find the formula for the Fermi velocity $v_F = \sqrt{2E_F/m}$ (which is the non-relativistic formula) in terms of fiducial values. The coefficient is a fiducial Fermi velocity.

e) From classical thermodynamics, we know that pressure

$$P = -\left(\frac{\partial E}{\partial V}\right)_{S,N}$$

where E is the sample internal energy, V is the sample volume, S is the sample entropy, N is the sample particle number, and the subscript S, N indicates the partial derivative is taken with entropy and particle number held constant. Since a free electron gas is confined by a confining potential, it must exert a counter potential on entities that confine it. In fact, by the correspondence principle of quantum mechanics, this counter potential can be assumed at the macroscopic level to a free electron gas pressure. The energy of the free electron gas is identifiable with the classical internal energy. Thus, we expect that a free electron gas exhibits a pressure derivable from the classical expression. Observation shows that this expectation is fulfilled. The pressure is called the degeneracy pressure, and its equation of state (i.e., pressure formula) is quite unlike that for an ideal gas. Derive the zero-temperature free-electron-gas pressure formula as a function of n_e. Then find the pressure formula in terms of fiducial values. **HINT:** The total energy of a sample is $NE_{\rm ave}$.

f) The bulk modulus of a material is a measure of its incompressibility or stiffness. The definition is

$$B = -V\left(\frac{\partial P}{\partial V}\right)_X = \rho\left(\frac{\partial P}{\partial \rho}\right)_X$$

where one assumes a constant mass and X stands for the thermodynamic variable held constant, either temperature or entropy (which can be held constant by adiabatic conditions). For ordinary solids and liquids, the difference between constant temperature and constant entropy is usually negligible. For a free electron gas at zero temperature, there is no difference.

The bulk modulus is actually a characteristic pressure for signficant volume or density change under a change pressure as can be seen by writing formula in the differential form

$$-\frac{dV}{V} = \frac{d\rho}{\rho} = \frac{dP}{B} .$$

If B were a constant (which it is not in any real case), then B would be the e-folding pressure: i.e., the pressure change required to change volume or density by a factor of e. The bigger the bulk modulus, the stiffer the substance.

Find the bulk modulus formula for the zero-tempature free electron gas. Then find the bulk modulus formula in terms of fiducial values.

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022 qfull 00200 2 5 0 moderate thinking: Fermi energies for free electron gas metals

Extra keywords: (Ha-324:2.3) volumes per atom 39.3, 23.0, 16.6 in A**3

3. The metals Na, Mg, and Al have, respectively 1, 2, and 3 free electrons per atom, standard atomic masses 22.98976928, 24.3050, and 26.9815386, and, under ordinary pressure and temperature, densities 0.968 g/cm^3, 1.738 g/cm^3, and 2.70 g/cm^3. What is the Fermi energy of these metals in electronvolts? Recall

$$E_F = \frac{\hbar^2}{2m}\left[\left(\frac{2}{g}\right)(3\pi^2)n_e\right]^{2/3}$$

$$= 3.06973\ldots \times 10^{-19}\,\mathrm{J} \times \left[\left(\frac{2}{g}\right) \frac{\rho}{1000\,\mathrm{kg/m^3}} \frac{50}{\mu_e}\right]^{2/3}$$

$$= 1.91597958\ldots\,\mathrm{eV} \times \left[\left(\frac{2}{g}\right) \frac{\rho}{1000\,\mathrm{kg/m^3}} \frac{50}{\mu_e}\right]^{2/3} \quad ,$$

where density is in MKS units.

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022 qfull 00210 1 3 0 easy math: free electron gas pressure

4. The pressure of a free electron gas (in three dimensions) is given by

$$P = \frac{2}{3}\mathcal{E} = \frac{\hbar^2}{2m}\left[3\pi^2\left(\frac{2}{g}\right)\right]^{2/3} \frac{2}{5}\left(\frac{\rho}{\mu_e m_{\mathrm{amu}}}\right)^{5/3} \quad ,$$

where $\mathcal{E}$ is the energy per unit volume and $g = 2$ for electron spin degeneracy. This result can be derived by using the classical 1st law of thermodynamics for $T = 0$ to relate P and $\mathcal{E}$ interpreted as the classical internal energy per unit volume. But it can also be derived from kinematics argument.

First note that a standing wave free electron eigenstate for one dimension of a infinite square well of length ℓ and wave number k

$$\psi = \sqrt{\frac{2}{\ell}}\sin(kx)$$

can be written as a superposition of oppositely traveling traveling wave states

$$\psi = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{1}{\ell}}e^{ikx} - \sqrt{\frac{1}{\ell}}e^{-ikx}\right) \quad ,$$

where have used the complex number definition of the sine function and dropped the global phase factor $1/i$ since it is physically irrelevant. Following the paradigm of quantum mechanics, it seems plausible to treat the standing wave state as literally a superposition of traveling wave states. One can generalize this idea to three dimensions. The traveling wave states can be thought of as continuously bouncing elastically off the walls of a 3-dimensional infinite square well and having their momentum component normal to wall inverted in the bounce. During the bounce, some kinetic energy becomes potential energy for a brief time. Perhaps, in real metals wave packets that are strongly peaked about stationary state $\vec{k}$ values are actually doing this. Textbooks grow coy on this point. But in any case, a classical interpretation of the traveling waves as particles bouncing off the walls of 3-dimensional infinite square well potential leads to the correct pressure result. One just says that the energy density of states per unit volume for $E \leq E_F$

$$\rho_E = \left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{g}{2}\frac{1}{4\pi^2}E^{-1/2}$$

is the density of classical particles in energy space per unit volume up to E_F and uses that density to calculate the pressure the particles exert.

Let's do the calculation.

a) If a (classical) particle of momentum magnitude p bounces elastically off a wall at an angel θ relative to the normal to the wall, what momentum is transferred to the wall in the normal direction? at angle

b) If you have a density of particles per unit (kinetic) energy per unit volume of ρ_E and the particle distribution in angle is isotropic, what is the density of particles per unit energy per unit volume per unit solid angle?

c) What is the flux of particles in per unit energy per unit area per unit solid angle?

d) What is the momemtum flux normal to the wall per unit area per unit energy per unit solid angle on the wall? Remember for a beam of particles coming in at angle to the wall of θ that cross-sectional area for the beam is $\cos\theta\,dA$, where dA is the area of wall the beam impinges on. For example, the cross-sectional area is $\theta = \pi/2$ is zero. A diagram might help you understand this cross-sectional area result.

e) Integrate the result from the part (d) answer over 2π solid angle about the normal to the wall and over all energy up the Fermi energy E_F to get the formula for the free electron gas pressure. Express the formula in terms of $\mathcal{E}$.

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022 qfull 00500 1 3 0 easy math: energy band structure function

Extra keywords: Bloch states

5. The energy band structure of the 1-dimensional Dirac comb solid is determined by the equation

$$\cos(Ka) = \cos(z) + \frac{\beta}{z}\sin(z) \ ,$$

where a is the cell size, K is the Bloch wavenumber, $z = ka \geq 0$ (where k is the wavenumber for a single cell), and

$$\beta = \frac{m\alpha a}{\hbar^2}$$

(where m is electron mass and α is the strength of the Dirac delta function potentials that make up the Dirac comb). The Bloch wavenumbers are quantized according to the rule

$$Ka = \frac{2\pi}{N}m \ ,$$

where $m = 0, 1, 2, 3, \ldots, N-1$ (where N is the number of cells). Actually, Ka is not determined to within an additive constant of 2π. Therefore one could also specify the range for m as

$$m = -\frac{N}{2}, -\frac{N}{2}+1, \ldots, \frac{N}{2}-1, \frac{N}{2}$$

since for N large one can with negligible error approximate N as even no matter what it actually is and add on an extra unphysical state. This second specification for m is more symmetrical and, as it turns out, makes k vary monotonically with K within a band. For definiteness in this problem, we assume $\beta \geq 0$.

The only possible solution z values are those that make confine

$$f(z) = \cos(z) + \frac{\beta}{z}\sin(z)$$

to the range $[-1, 1]$. For a Ka value, one solves

$$\cos(Ka) = f(z)$$

for ka and then k. Thus, the k values have a non-trivial quantization rule. The energy of the k state is then determined by

$$E = \frac{\hbar^2 k^2}{2m} \ .$$

The energies have a non-trivial quantization rule too.

A key point is the function $f(z)$ can oscillate above 1 and below -1 and in those regions there are no solutions for k, and therefore no allowed states and no solutions for E. Those energy regions are the famous energy gaps. The allowed regions are the energy bands. Since N

is an enormous number for macroscopic samples, the energy bands are very dense in number of states and one gets states virtually to the z points where $|f(z)| = 1$. The z values that yield $|f(z)| = 1$ are the band limits. Each band has a start and end limit. There are corresponding energy start and end limits.

a) Determine the formula end limit of a general ℓth energy band. Note $\ell = 1, 2, 3, \ldots$ Show that the formula is the end limit formula and never gives start limits. **HINT:** Finding the formula is easy. Showing that it is the end limit requires taking the derivative of $f(z)$.

b) A key point to proof is that there is only one limit point between two consecutive end limit points given by the formula in the part (a). This single limit point is a start limit point.

In a test situation just assume there is a single start limit point between the end limit points and go onto the rest of the problem.

In a non-test situation, do the proof. **HINT:** Prove there is a single stationary point between the consecutive end limit points. The function $f(z)$ value at the stationary point is must be outside of the range $[-1, 1]$ by the part (a) answer. Also from the part (a) answer, the function at the stationary point must be greater than 1 if the next end limit point $f(z) = -1$ and the function at the stationary point must be less than 1 if the next end limit point is $f(z) = 1$ Thus from the stationary point to the next end limit point the function is is monotonic and crosses into the allowed range once only. That is crossing is the start limit point itself. The stationary point itself can't be found analytically in general, but its uniqueness can be proven by arranging the equation for stationary point into a form where $\tan(z)/z$ equals something.

c) Find an approximate formula for the start limit for the first band in the limit that β is very large. Show that this formula also gives the start limit for $\beta = 0$, and thus constitutes an interpolation formula: a formula that gives correct limiting behavior and interpolates smoothly in between those limits. **HINT:** Set the function $f(z)$ equal to 1 and expand the trigonometric functions in $f(z)$ about π to 1st order in small $z-\pi$. Why are the expansions the good thing to do and why is it good not to expandi the $1/z$ factor to 1st order in small $z - \pi$ even though it would be consistent with the other expansions?

d) Find an approximate formula for the start limit $\Delta z = z - z_{\ell-1} = z - (\ell - 1)\pi$ for the general ℓth band, except that $\ell \geq 1$. **HINT:** Set $f(z) = (-1)^{\ell-1}$ and expand $\cos(z)$ to second order in small Δz about $z_{\ell-1}$. and $\sin(z)$ to 3rd order in small Δz about $z_{\ell-1} = (\ell-1)\pi$ Do **NOT** approximate $1/(z_{\ell-1} + \Delta z$. Write $\beta = yz_{\ell-1}/2$ as a simplification. What approximate size limit must be put on Δz for our approximations to be valid? What is Δz in the limit that $z_{\ell-1}$ becomes very large.

e) Take the interpolation formula from the part (c) answer the Δz formula for very large $z_{\ell-1}$ from the part (d) answer and invent an interpolation formula for Δz valid for all ℓ. We mean it is valid for ℓ in that it gives the right limiting behavior for β for the $\ell = 1$ and the right limiting behaviro for ℓ becoming very large. Since it has those right limiting behaviors, it may well interpolate to some accuracy everywhere. **HINT:** There is no absolutely right answer, but a fairly obvious interpolation formula leaped to yours truly's eye.

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022 qfull 00510 1 3 0 easy math: energy band structure function 2

6. This a super-easy problem if you can understand the lengthy setup.

For the 1-dimensional Dirac comb potential, the band structure is determined by the equation

$$\cos(Z) = f(z) ,$$

where

$$f(z) = \cos(z) + \frac{\beta}{z}\sin(z) .$$

The Z is determined by the Bloch wavenumber quantization rule

$$Z = Ka = \frac{2\pi}{N}m \qquad \text{where } m = 0, 1, 2, \ldots, (N-1)$$

where N is the number of number of cells and a is the cell length. For a macroscopic system N is huge, and so Z can be close to any real number in the range $[0, 2\pi]$. The $z = ka$, where k is the ordinary wavenumber from which the energy of a single-particle state can be determined from

$$E = \frac{\hbar^2 k^2}{2m} \ .$$

If we knew a z value, determining the corresponding Z value would be a cinch. But we know the Z values and need to determine the z values. There is no analytic solution for general z.

We do know that the only solutions are in bands set by the fact that $\cos(Z)$ can only be in the range $[-1, 1]$. From earlier work, we know that

$$z_{\ell,\text{start}} = (\ell - 1)\pi + \Delta z_\ell = (\ell - 1)\pi + \frac{2\beta\pi}{2\beta + 4 + \pi^2(\ell - 1)}$$

is a good approximation for the start limit of band ℓ and

$$z_{\ell,\text{end}} = \ell\pi$$

is the exact result for the end limit of a band ℓ. The band numbers run form $\ell = 1$ to $\ell = \infty$. The $\cos(Z)$ value sweeps from 1 to -1 as z increases for odd bands and from -1 to 1 for even bands.

Let's define a parameter g that runs from 0 to 1 and parameterize Z in terms of g thusly

$$Z = \begin{cases} g\pi & \text{for } \ell \text{ odd;} \\ (g+1)\pi & \text{for } \ell \text{ even.} \end{cases}$$

Using g (which we can easily find for any Z value and any ℓ) and the formulae for $z_{\ell,\text{start}}$ and $z_{\ell,\text{end}}$ devise an approximate z formula that is **LINEAR** in g. **HINT:** This is super-easy, but you should test that $g = 0$ and $g = 1$ give the correct band limits: $z(\ell, g = 0) = z_{\ell,\text{start}}$ and $z(\ell, g = 1) = z_{\ell,\text{end}}$.

Chapt. 23 Statistical Mechanics

Multiple-Choice Problems

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023 qmult 00240 1 1 3 easy memory: statistical weight formulae
Extra keywords: See Gr-234–235

1. The formulae

$$W = N!\prod_i \frac{g_i^{N_i}}{N_i!} \ , \qquad W = \prod_i \binom{g_i}{N_i} \ , \qquad W = \prod_i \binom{g_i - 1 + N_i}{N_i} \ ,$$

are statistical weights for, respectively,

a) identical fermions, distinct particles, identical bosons.
b) distinct particles, identical bosons, identical fermions.
c) distinct particles, identical fermions, identical bosons.
d) identical bosons, distinct particles, identical fermions.
e) distinct particles, identical flimsions, identical bozos.

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023 qmult 00350 1 4 5 easy deducto-memory: Stirling's series
Extra keywords: mathematical physics

2. "Let's play *Jeopardy*! For \$100, the answer is:

$$\ln(z!) = z\ln(z) - z + \frac{1}{2}\ln(z) + \frac{1}{2}\ln(2\pi) + \frac{1}{12z} - \frac{1}{360z^3} + \frac{1}{1260z^5}$$

which is an asymptotic series that is increasingly accurate as $z \to \infty$, but is not so bad even for z as small as 1."

What is ____________ series, Alex?

a) the ICE b) Wankel's c) Diesel's d) Carnot's e) Stirling's

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023 qmult 00330 1 4 1 easy deducto-memory: Lagrance multipliers
Extra keywords: mathematical physics

3. "Let's play *Jeopardy*! For \$100, the answer is: It is a method for finding the constrained stationary points of a multi-variable function."

What is ____________, Alex?

a) Lagrange multipliers b) the Stirling approximation c) Stirling's series
d) the Maxwell-Boltzmann distribution e) the Fermi-Dirac distribution

---

023 qmult 00340 1 1 3 easy memory: Lagrange multiplier formula for W

4. The formula

$$h = \ln(W) + \alpha\left(\sum_i N_i - N\right) + \beta\left(\sum_i N_i E_i - E\right)$$

can be used to find the N_i values that maximize value of W subject to the constraints:

a) $\sum_i N_i E_i = E$ and all $N_i \geq 0$. b) $\sum_i N_i = N$ and all $N_i \geq 0$.
c) $\sum_i N_i = N$ and $\sum_i N_i E_i = E$. d) $\sum_i N_i = N$ and $W \geq 0$.
e) $\sum_i N_i = N$ and $W \leq 0$

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023 qmult 00352 1 1 5 easy memory: ln of factorials difference

5. The difference

$$\ln(z!) - \ln[(z-1)!]$$

equals:

a) $\ln(z-1)$. b) $\ln(z!)$. c) $z-1$. d) z. e) $\ln(z)$.

---

023 qmult 00410 1 1 2 easy memory: stat mech entropy

6. The formula

$$S = k \ln(W)$$

is the statistical mechanics formula for:

a) statistical weight. b) entropy. c) energy.
d) the Maxwell-Boltzmann distribution. e) the Fermi-Dirac distribution.

---

023 qmult 00490 1 1 4 easy memory: stat mech distribution formulae

Extra keywords: GR-241

7. The formulae

$$f = e^{-(E-\mu)/(kT)} \; , \qquad f = \frac{1}{e^{(E-\mu)/(kT)} + 1} \; , \qquad f = \frac{1}{e^{(E-\mu)/(kT)} - 1}$$

are, respectively, ________________________________ distributions. These distribution give the factional occupation a state of energy E in thermodynamic equilibrium.

a) Maxwell-Boltzmann, Bose-Einstein, Fermi-Dirac
b) Maxwell-Boltzmann, Fermi-Einstein, Bose-Dirac
c) Maxwell-Dirac, Fermi-Einstein, Bose-Boltzmann
d) Maxwell-Boltzmann, Fermi-Dirac, Bose-Einstein
e) Maxwell-Bose, Fermi-Einstein, Boltzmann-Dirac

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023 qmult 00530 1 1 1 easy memory: MB average energy per particle

8. The factorial function definition is

$$z! = \int_0^\infty t^z e^{-t} \, dt \; .$$

It is easily shown that

$$z! = z(z-1)! \; .$$

The formula gives

$$z! = n!$$

for $z = n$ an integer greater than or equal to zero and $(-1/2)! = \sqrt{\pi}$. The values for z a negative integer are undefined. Using the factorial function or otherwise find the **AVERAGE PARTICLE ENERGY** for a system of particles obeying the Maxwell-Boltzmann distribution and having density of states per energy per volume proportional to $E^{1/2}$ (which the energy factor for the density of states in an 3-dimensional infinite square containing free particles).

a) $E_{\text{ave}} = \frac{3}{2}kT$ b) $E_{\text{ave}} = \frac{1}{2}kT$ c) $E_{\text{ave}} = kT$ d) $E_{\text{ave}} = \frac{3}{5}E_{\text{Fermi}}$
e) $E_{\text{ave}} = E_{\text{Fermi}}$

---

023 qmult 00540 1 1 1 easy memory: Maxwell-Boltzmann chemical potential

Extra keywords: Need the factorial function, and so give question 530 first.

9. Given the distribution function

$$f = e^{-(E-\mu)/(kT)}$$

which gives the fractional occupation of any state and

$$dg_{\text{total}} = \frac{g}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}\,dE$$

(which is the differential degeneracy of states per unit volume in single-particle energy interval dE in the continuum approximation for a 3-dimensional infinite square well containing free particles of mass m and internal degeneracy g) solve for the chemical potential μ. The density of particles is n.

a) $\mu = kT\ln\left\{\frac{n}{g\left[mkT/\left(2\pi\hbar^2\right)\right]^{3/2}}\right\}$ b) $\mu = kT\ln\left\{\frac{n}{g\left[2mkT/\left(\pi\hbar^2\right)\right]^{3/2}}\right\}$

c) $\mu = \ln\left\{\frac{n}{g\left[mkT/\left(2\pi\hbar^2\right)\right]^{3/2}}\right\}$ d) $\mu = kT\ln\left\{\frac{n}{g\left[(3/2)mkT/\left(\pi\hbar^2\right)\right]^{3/2}}\right\}$

e) $\mu = \ln\left\{\frac{n}{g\left[2mkT/\left(\pi\hbar^2\right)\right]^{3/2}}\right\}$

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023 qmult 00820 1 1 3 easy memory: Planck law

10. The specific intensity formula

$$B_\nu = \frac{2h\nu^3}{c^2}\frac{1}{e^{h\nu/(kT)}-1}$$

is for a thermodynamic equilibrium:

a) Maxwell-Boltzmann gas. b) Fermi-Dirac gas c) photon gas. d) fermion gas.
e) distinct particle gas.

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023 qmult 00830 1 1 2 easy memory: hohlraum

11. A hohlraum is a cavity where the wall and radiation field are in thermodynamic equilibrium. A small hole in the wall allows the radiation field to be observed with minimal perturbation of the radiation field. The emission from the hole is a nearly perfect:

a) Fermi-Dirac gas. b) blackbody spectrum. c) Bose-Einstein condensate.
d) superfluid liquid. e) Maxwell-Boltzmann gas.

---

023 qmult 00840 1 1 3 easy memory: Wien's law

12. The Planck law in the wavelength version is

$$B_\lambda = \frac{2hc^2}{\lambda^5}\frac{1}{e^{hc/(\lambda kT)}-1} .$$

The **SHORT**-wavelength approximation to this formula is Wien's law:

a) $\frac{kTc}{\lambda^4}$. b) $\frac{2kTc}{\lambda^4}$. c) $\frac{2hc^2}{\lambda^5}e^{-hc/(\lambda kT)}$. d) $\frac{kTc}{2\lambda^4}$. e) $\frac{2hc^2}{\lambda^5}e^{hc/(\lambda kT)}$.

---

023 qmult 00842 1 1 2 easy memory: Rayleigh-Jeans law

13. The Planck law in the wavelength version is

$$B_\lambda = \frac{2hc^2}{\lambda^5}\frac{1}{e^{hc/(\lambda kT)} - 1} \ .$$

The **LONG**-wavelength approximation to this formula is Wien's law:

a) $\dfrac{kTc}{\lambda^4}$. b) $\dfrac{2kTc}{\lambda^4}$. c) $\dfrac{2hc^2}{\lambda^5}e^{-hc/(\lambda kT)}$. d) $\dfrac{kTc}{2\lambda^4}$. e) $\dfrac{2hc^2}{\lambda^5}e^{hc/(\lambda kT)}$.

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023 qmult 00850 1 1 1 easy memory: approximate solution Planck law stationary points

14. The function

$$f(x) = \frac{x^p}{e^x - 1}$$

for $x \geq 0$ and $p >> 1$ has the approximate maximizing value:

a) p. b) $p/2$. c) $1/p$. d) p^2. e) $\ln(p)$.

Full-Answer Problems

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023 qfull 00140 1 3 0 easy math: the MB FD BE distributions derived

1. Consider a system consisting of quantized single-particle states and fixed total number of particles N and fixed total energy E. We make the approximation that particles can occupy only one single-particle state at time: i.e., they are not in superpositions of single-particle states. The overall microscopic state of the system is set by specifying arrangement of the particles in the single-particle states. Note that exchanging distinct particles changes the microscopic state and exchanging identical particles does not.

   The set of single-particle states of the same energy E_i can be called an energy level—a term which is used in different ways in different contexts. The number of single-particle states in an energy level i is the energy level degeneracy g_i. A configuration is the set of occupation numbers $\{N_i\}$ for the energy levels of the system. The statistical weight W of a configuration is the number of distinct microscopic states that correspond to that configuration.

   The fundamental axiom of statistical mechanics is that in thermodynamic equilibrium all the microscopic states are equally probable. Thermodynamic equilibrium for a system occurs when the system is not changing thermodynamically with time at the macroscopic level. In thermodynamic equilibrium, the initial conditions of the system no longer determine its macroscopic behavior and their signature in the system has been effectively erased.

   The fundamental axiom implies that probability distribution for the configuration is just the normalized statistical weights and the most probable configuration is the one with the largest statistical weight. It turns out the probability distribution given by the statistical weights is extremely peaked around the most probable configuration for systems of macroscopically large numbers of particles. The macroscopic thermodynamic equilibrium state is essentially this most probable configuration. The natural logarithm the statistical weight times Boltzmann's constant k identified with the classical entropy which maximizes for thermodynamic equilibrium. Thus we have

$$S = k\ln(W) \ .$$

   a) The statistical weight for the configuration for a system with distinct particles is

$$W = N!\prod_i \frac{g_i^{N_i}}{N_i!} \ .$$

Solve for the set of N_i that maximize the statistical weight subject to the constraints

$$N = \sum_i N_i \ , \qquad E = \sum_i N_i E_i \ , \qquad N_i \geq 0 \ .$$

For conventional reasons, the Lagrange multiplier for the particle number constraint should be label α and that for the energy constraint β. Use appropriate approximations to get a simple analytic formula for a maximizing N_i in which the degeneracy g_i occurs only as a leading coefficient. What is the function with the degeneracy factor suppressed and what is it called?

b) The statistical weight for the configuration for a system with identical fermions is

$$W = \prod_i \binom{g_i}{N_i} \ .$$

Repeat the requirements from part (a) for this statistical weight.

c) The statistical weight for the configuration for a system with identical bosons is

$$W = \prod_i \binom{g_i - 1 + N_i}{N_i} \ .$$

Repeat the requirements from part (a) for this statistical weight.

d) The lagrange multiplier function has an uncontrained stationary point at the maximizing values of N_i. This fact along with the 1st law of classical thermodynamics

$$dE = T\,dS - \mu\,dN$$

for the case of fixed volume but variable entropy and particle number (T being temperature and μ being the chemical potential) and the identificiation of entropy allows α and β to be determined in terms of classical thermodynamics variables. Make the determinations.

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023 qfull 00440 1 3 0 easy math: photon gas the full story

2. Photons in thermodynamic equilibrium with some container or with some gas of massive particles can be thought as a photon gas obeying Bose-Einstein statistics. Photons are extreme relativistic particles, but nevertheless the simple formalism for the statistical mechanics of non-relativistic systems still applies with some modifications:

1) The energies of quantized single-particle states are related to the momentum, frequency, wavelength, and wavenumber of the state by

$$E = pc = h\nu = \frac{hc}{\lambda} = \hbar ck \ .$$

Note that above expression embodies the de Broglie formula $p = h/\lambda$ which de Broglie took from photons and applied to massive particles—but with the difference that massive particles in the non-relativistic limit relate kinetic energy to momentum by $E = p^2/(2m)$.

2) Photons are spin-1 bosons, but for some reason only the $m = \pm 1$ states are allowed. Thus, the each spatial quantized single state has a degeneracy of $g = 2$.

3) The number of photons is not conserved. The unspecified processes that transform one overall microscopic quantum state to another can create and destroy photons. Thus, photon gas will relax to a maximum entropy state with no constraint on total photon number. This means that the Lagrange multiplier $\alpha = \mu/kT$ is zero.

Let's see what we can learn about the thermodynamic equilibrium photon gas.

a) Given that periodic boundary conditions for a 3-dimensional infinite well rectangular box and ℓ for the length of a general dimension, the wavenumber of single-particle states for this dimension is quantized according to the rule

$$k\ell = 2\pi n \ , \qquad \text{where} \qquad n = 0, \pm 1, \pm 2, \pm 3, \ldots \ .$$

What is the density of states in phase space which is the product of k-space and space space? Do not forget the internal degeneracy factor g.

b) Given the Bose-Einstein distribution

$$f = \frac{1}{e^{(E-\mu)/(kT)} - 1}$$

(where E is single-particle state energy, μ is chemical potential, and T is temperature), find the formula for the energy density per unit frequency $\mathcal{E}_\nu$ for the thermodynamic equilibrium photon gas. Note energy density per unit frequency, **NOT** photon number density per unit frequency.

c) In radiative transfer it is customary to work with specific intensity B_ν rather than $\mathcal{E}_\nu$. The specific intensity is the energy flux (energy per unit area perpendicular to the direction of motion per unit time) per unit frequency per unit solid angle. Find the formula for B_ν.

d) Find the frequency integrated formula for B_ν: i.e., find B. Note that the factorial function is

$$z! = \int_0^\infty t^z e^{-t}\,dt = \begin{cases} z(z-1)! & \text{for general complex } z\text{, except for } z \text{ a negative integer;} \\ \pm\infty & \text{for } z \text{ a negative integer;} \\ n! & \text{for } n \text{ an integer with } n \geq 0; \\ \sqrt{\pi} & \text{for } z = -1/2 \end{cases}$$

(Ar-453), that the Riemann zeta function defined as an infinite sum (convergent for $\mathrm{Re}(z) > 1$) is

$$\zeta(z) = \sum_{\ell=1}^{\infty} \frac{1}{\ell^z} = \begin{cases} \dfrac{\pi^2}{6} & \text{for } z = 2; \\ \dfrac{\pi^4}{90} & \text{for } z = 4; \\ \dfrac{\pi^8}{945} & \text{for } z = 6, \end{cases}$$

(Ar-282, 285) and that the Stefan-Boltzmann constant is

$$\sigma = \frac{2\pi^5}{15}\frac{k^4}{h^3c^2} = 5.670400(40) \times 10^{-8}\,\mathrm{W\,m^{-2}\,K^{-4}} \ .$$

Also find the total energy per unit volume. Note that the radiation constant

$$a = \frac{4\sigma}{c} = 7.5657 \times 10^{-16}\,\mathrm{J\,m^{-3}\,K^{-4}} \ .$$

e) The energy flux from a surface emitting like an exact blackbody is given by

$$F = \int_{2\pi} B \cos\theta \, d\Omega \ ,$$

where the integral is over 2π solid angle and we have assumed the z direction is the outward normal direction from the surface. The $\cos\theta$ factor decrease in area perpendicular to a beam through an opening in the surface. For example, if $\theta = \pi/2$, there would be no emission through the opening. Evaluate the formula for F.

f) What is the formula for B_λ: i.e., the specific intensity as a function of wavelength rather than μ. Note

$$B_\lambda \, d\lambda = B_\nu \, d\nu \ .$$

g) The Wein approximation (derived 1896) is the approximate formula for B_λ in the limit of small wavelength. The Rayleigh-Jeans law (derived 1900–1905) is the approximate formula for B_λ in the limit of large wavelength. Derive these two approximate formulae from the exact formula for B_λ found in the part (f) answer.

h) What is an iteration formula for the maximizing point of functions of the form

$$f(x) = \frac{x^p}{e^x - 1} \ ,$$

where $p > 1$? What is a good initial value x_0 for the iteration and is the iteration guaranteed to converge?

i) Find the formulae for the maximizing ν and λ values for, respectively, B_ν and B_λ. You only need to find the coefficients of formulae approximately, but if you are ambitious a small computer code will allow you do find the coefficients to machine accuracy. Then give Wien's law (AKA Wien's displacement law).

Chapt. 24 Interaction of Radiation and Matter

Multiple-Choice Problems

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024 qmult 00100 1 1 4 easy memory: Maxwell's equations

1. Classical electrodynamics is summarized in:
   - a) Stirling's formula.
   - b) Heitler's five equations.
   - c) Montefeltro's three laws.
   - d) Maxwell's four equations.
   - e) Euclid's axioms.

---

024 qmult 00200 1 4 5 easy deducto-memory: EM potentials

2. "Let's play *Jeopardy*! For \$100, the answer is:

$$\vec{E} = -\nabla\Phi - \frac{1}{c}\frac{\partial\vec{A}}{\partial t} \qquad \text{and} \qquad \vec{B} = \nabla\times\vec{A}\ .\text{''}$$

   - a) What are Maxwell's equations, Alex?
   - b) What are two arbitrary equations, Alex?
   - c) What are the gauge transformation equations, Alex?
   - d) What are the Noman equations, Alex?
   - e) What are the equations for deriving the electromagnetic fields from the electromagnetic potentials, Alex?

---

024 qmult 00300 1 1 3 easy memory: transverse gauge

3. The condition imposed for the transverse gauge (or radiation or Coulomb gauge) is:
   - a) $\nabla\cdot\vec{B} = 0$.
   - b) $\nabla\cdot\vec{A} + (1/c)\partial\Phi/\partial t = 0$.
   - c) $\nabla\cdot\vec{A} = 0$.
   - d) $\vec{A}' = \vec{A} + \nabla\Lambda$.
   - e) $\Phi' = \Phi - (1/c)\partial\Lambda/\partial t$.

---

024 qmult 00400 1 4 2 easy deducto-memory: EM energy density

Extra keywords: Reference Ja-236

4. "Let's play *Jeopardy*! For \$100, the answer is:

$$\mathcal{E} = \frac{E^2 + B^2}{8\pi}\ .\text{''}$$

   - a) What Laplace's equation, Alex?
   - b) What the energy density of the electromagnetic field in SI units, Alex?
   - c) What the energy density of the electromagnetic field in Gaussian units, Alex?
   - d) What Poynting's vector, Alex?

e) What is an example of using "E" for two quantities in one equation, Alex?

---

024 qmult 00500 1 1 2 easy memory: wave equation solution

5. The simple wave equation

$$\nabla^2\vec{g} = \frac{1}{c}\frac{\partial^2\vec{g}}{\partial t^2}$$

has a very general solution of the form:

a) $\vec{g} = 0$.
b) $\vec{g}(\vec{k}\cdot\vec{r} - \omega t)$, where $\vec{g}$ is any vector function and $\omega = |\vec{k}|c$.
c) $\vec{g}(\vec{k}\times\vec{r} - \omega t)$, where $\vec{g}$ is any vector function and $\omega = |\vec{k}|c$.
d) $\vec{g}(\omega t)$.
e) $\vec{g}(\vec{k}\cdot\vec{r})$.

---

024 qmult 00600 1 1 2 easy memory: EM perpendicular vectors

6. For self-propagating electromagnetic radiation the electric field, magnetic field, and propagation directions are:

a) collinear.
b) mutually perpendicular.
c) self-perpendicular.
d) arbitrary.
e) random.

---

024 qmult 00700 1 4 4 easy deducto-memory: box quantization

7. "Let's play *Jeopardy*! For $100, the answer is: A standard trick in quantum mechanics for replacing basically isotropic, homogeneous systems with complex boundary conditions by a simpler, tractable, periodic-boundary-condition system which—according to the faith—must have the same bulk properties."

a) What is nothing I've ever heard of, Alex?
b) What is the tethered function method, Alex?
c) What is black magic, Alex?
d) What is box quantization, Alex?
e) What is the way to get a completely wrong answer, Alex?

---

024 qmult 00800 1 4 3 easy deducto-memory: interaction Hamiltonian

8. "Let's play *Jeopardy*! For $100, the answer is:

$$H = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 + e\Phi + V \text{ .''}$$

a) What is Schrödinger's equation, Alex?
b) What is the Hamiltonian for the simple harmonic oscillator, Alex?
c) What is the particle Hamiltonian including the interaction with the electromagnetic field, Alex?
d) What is the interaction Hamiltonian of the electromagnetic field, Alex?
e) What is any old Hamiltonian, Alex?

---

024 qmult 01200 1 1 4 easy memory: cross section

9. What one often wants from a radiation interaction calculation is a coefficient or the like that can be employed in macroscopic radiative transfer: e.g.,

a) a postulate.

b) a postulant.
c) a golden section.
d) a cross section.
e) a crossbow.

---

024 qmult 01300 1 1 1 easy memory: quantizing radiation

10. To quantize the electromagnetic radiation field we assert that the energy of radiation mode cannot take on a continuum of values, but must come in:

a) integral amounts of a basic unit called a quantum of electromagnetic radiation or a photon.
b) amounts related by the golden section.
c) photoids.
d) integral numbers of ergs.
e) integral numbers of eVs.

---

024 qmult 01400 1 1 3 easy memory: creation and annihilation operators

11. The electromagnetic field operator is defined in terms of:

a) Bell and Sprint operators.
b) left and right operators.
c) creation and annihilation operators.
d) procreation and inhibition operators.
e) genesis and revelations operators.

---

024 qmult 01500 1 1 2 easy memory: zero point energy

12. In the formalism of quantized electromagnetic radiation, the fact that the creation and annihilation operators don't commute leads to:

a) nothing in particular.
b) the existence of zero-point energy.
c) energy less than the zero-point energy.
d) living close to the office.
e) living in the office.

---

024 qmult 01600 1 4 4 easy deducto-memory: Einstein stimulated em.

13. "Let's play *Jeopardy*! For \$100, the answer is: An effect discovered by Einstein by means of a thermodynamic equilibrium detailed balance argument."

What is ____________, Alex?

a) spontaneous emission b) special relativity c) the photoelectric effect
d) stimulated emission e) spontaneous omission

---

024 qmult 01700 1 4 5 easy deducto-memory: free particles don't radiate

14. "Let's play *Jeopardy*! For \$100, the answer is: A particle that cannot radiate by a Fermi golden rule process in the non-relativistic limit and perhaps not at all—but one never knows what special exotic cases may be said to allow it to radiate."

a) What is a classical particle, Alex?
b) What is a neutral pion, Alex?
c) What is a quark, Alex?
d) What is an unbound particle subject to potentials, Alex?
e) What is a free particle, Alex?

---

024 qmult 01800 1 1 1 easy memory: conservation of momentum

15. Since it seems that no quantum mechanical matter particle can actually be in a pure momentum eigenstate, conservation of momentum in radiative emission or absorption in the instructor's view

    a) cannot be strict in a classical sense.
    b) can be strict in a classical sense.
    c) both can and cannot be strict in a classical sense.
    d) can neither be nor not be strict in a classical sense.
    e) is moot and categorically valid in a classical sense.

---

024 qmult 01900 1 1 2 easy memory: electric dipole transitions

16. Typically, strong atomic and molecular transitions are ____________ transitions.

    a) electric quadrupole b) electric dipole c) magnetic dipole
    d) electric monopole e) magnetic metropole

---

024 qmult 02000 1 4 4 easy deducto-memory: selection rules

17. "Let's play *Jeopardy*! For \$100, the answer is: The selection rules for electric dipole transitions (i.e., allowed transitions) between energy eigenstates whose angular parts are spherical harmonics."

    a) What are Hund's rules, Alex?
    b) What are $\Delta m = \pm 2$ and $\Delta\ell = 0$, Alex?
    c) What are $\Delta m = \pm 1$ and $\Delta\ell = 0$ or ± 1, Alex?
    d) What are $\Delta m = 0$ or ± 1 and $\Delta\ell = \pm 1$, Alex?
    e) What are taking the fresher and firmer ones, Alex?

Full-Answer Problems

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024 qfull 00300 2 5 0 moderate thinking: classical EM scattering

Extra keywords: reference Mi-83

1. Say we had a classical simple harmonic oscillator (SHO) consisting of a particle with mass m and charge e and a restoring force $m\omega_0^2$ where ω_0 is the simple harmonic oscillator frequency. This SHO is subject to driving force caused by traveling electromagnetic field (i.e., light):

$$\vec{F}_{\text{drive}} = e\vec{E}_0 e^{i\omega t} \ ,$$

where $\vec{E}_0$ is the amplitude, ω is the driving frequency, and we have used the complex exponential form for mathematical convenience: the real part of this force is the real force. The magnetic force can be neglected for non-relativistic velocities. The Lorentz force is

$$\vec{F} = e\left(\vec{E} + \frac{\vec{v}}{c} \times \vec{B}\right)$$

(Ja-238) and $\vec{E}$ and $\vec{B}$ are comparable in size for electromagnetic radiation, and so the magnetic force is of order v/c smaller than the electric force. (See also MEL-130.) An oscillating charge is an accelerating charge and will radiate electromagnetic radiation. The power radiated classically is

$$P = \frac{2e^2a^2}{3c^3} \ ,$$

where $\vec{a}$ is the charge acceleration. This radiation causes an effective damping force given approximately by

$$\vec{F}_{\text{damp}} = -m\gamma\vec{v} \ ,$$

where

$$\gamma = \frac{2e^2\omega_0^2}{3mc^3} .$$

The full classical equation of motion of the particle is

$$m\vec{a} = -m\omega_0^2\vec{r} + e\vec{E}_0 e^{i\omega t} - m\gamma\vec{v} .$$

a) Solve the equation of motion for $\vec{r}$ and $\vec{a}$. **HINTS:** The old trial solution approach works. Don't forget to take the real parts although no need to work out the real part explicitly: i.e., Re[solution] is good enough for the moment.

b) Now solve for the time average of the power radiated by the particle. **HINT:** You will need the explicit real acceleration now.

c) The average power radiated must equal the average power absorbed. Let's say that the particle is in radiation flux from a single direction with specific intensity

$$I_0 = \frac{cE_0^2}{8\pi}$$

(Mi-9), where time averaging is assumed *como usual.* The power absorbed from this flux is $\sigma(\omega)I_0$, where $\sigma(\omega)$ is the cross section for energy removed. Solve for $\sigma(\omega)$ and then find show that it can be approximated by a Lorentzian function of ω with a coefficient $\pi e^2/(mc)$. **HINT:** It is convenient to absorb some of the annoying constants into another factor of γ.

d) Now rewrite the cross section as a function of $\nu = \omega/(2\pi)$ (i.e., the ordinary frequency) and then integrate over ν to get the frequency integrated cross section $\sigma_{\nu\ \rm int}$ of the system. What is the remarkable thing about $\sigma_{\nu\ \rm int}$? Think about how it relates to the system from which we derived it. Evaluate this frequency integrated cross section for an electron. **HINT:** The following constants might be useful

$$\alpha = \frac{e^2}{\hbar c} = \frac{1}{137.036} , \qquad \hbar = 1.05457 \times 10^{-27}\,\text{erg}\,\text{s} , \qquad \text{and} \qquad m_e = 9.10939 \times 10^{-28}\,\text{g} .$$

---

024 qfull 00500 2 5 0 moderate thinking: gauge invariance

Extra keywords: (Ba-299:1)

2. The gauge transformations of the electromagnetic potentials are:

$$\vec{A}(\vec{r},t)' = \vec{A}(\vec{r},t) + \nabla\chi(\vec{r},t)$$

and

$$\phi(\vec{r},t)' = \phi(\vec{r},t) - \frac{1}{c}\frac{\partial\chi(\vec{r},t)}{\partial t}$$

(Ja-220), where $\vec{A}(\vec{r},t)$ is the vector potential, $\phi(\vec{r},t)$ is the scalar potential, the primed quantities are the transformed versions, and $\chi(\vec{r},t)$ is the gauge. Show that the solution to the time-dependent Schrödinger equation for n particles of charge e and mass m transforms so

$$\Psi(\vec{r}_1,\ldots,\vec{r}_n,t)' = \exp\left[\frac{ie}{\hbar c}\sum_{i=1}^{n}\chi(\vec{r}_i,t)\right]\Psi(\vec{r}_1,\ldots,r_n,t)$$

under a gauge transformation of the potentials treated as classical fields: i.e., if Ψ' satisfies a primed version of the Schrödinger equation, then Ψ satisfies an unprimed version. **HINT:** It suffices to consider one particle in one dimension. I know of no simplifying tricks. You just have to grind out the 15 odd terms very carefully.

---

024 qfull 00700 2 5 0 moderate thinking: QM CA operators

Extra keywords: (Ba-299:3)

3. The photon creation and destruction operators of the electromagnetic field photons (the CA operators for short) are defined by, respectively

$$A^\dagger_{\vec{k}\vec{\lambda}}|\ldots,N_{\vec{k}\vec{\lambda}},\ldots\rangle=\sqrt{\frac{2\pi\hbar c^2}{\omega}}\sqrt{N_{\vec{k}\vec{\lambda}}+1}|\ldots,N_{\vec{k}\vec{\lambda}}+1,\ldots\rangle$$

and

$$A_{\vec{k}\vec{\lambda}}|\ldots,N_{\vec{k}\vec{\lambda}},\ldots\rangle=\sqrt{\frac{2\pi\hbar c^2}{\omega}}\sqrt{N_{\vec{k}\vec{\lambda}}}|\ldots,N_{\vec{k}\vec{\lambda}}-1,\ldots\rangle\ ,$$

where $N_{\vec{k}\vec{\lambda}}$ is the number of photons in the box quantization mode specified by wavenumber $\vec{k}$ and polarization vector $\vec{\lambda}$. All the physically unique states created by these operators are assumed to be orthogonal. From this assumption it follows that creation and annihilation operators are Hermitian conjugates as their labeling indicates: we'll leave that proof *sine die.* The annihilation operator acting on the empty mode (i.e., one with $N_{\vec{k}\vec{\lambda}}=0$) gives a zero or null state (or vector). Any operator acting on a zero state gives a zero state, of course. Thus, non-zero commutator identities can't be proven by acting on zero states and it is understood that zero states are never thought of in proving commutator identities.

Dimensionless forms of these operators are, respectively,

$$a^\dagger_i|\ldots,N_i,\ldots\rangle=\sqrt{N_i+1}|\ldots,N_i+1,\ldots\rangle$$

and

$$a_i|\ldots,N_i,\ldots\rangle=\sqrt{N_i}|\ldots,N_i-1,\ldots\rangle\ ,$$

where index i subsumes both the $\vec{k}$ and $\vec{\lambda}$ indices.

a) Prove the commutator identities

$$[a_i,a_j]=0\ ,\qquad [a^\dagger_i,a^\dagger_j]=0\qquad\text{and}\qquad [a_i,a^\dagger_j]=\delta_{ij}\ .$$

Remember the case of $i=j$ for the first two identities. What are the dimensioned forms of these commutator identities?

b) Recall that classically the total energy in the radiation field is

$$\mathcal{E}=\int\left(\frac{E^2+B^2}{8\pi}\right)d\vec{r}\ ,$$

where calligraphic $\mathcal{E}$ is total energy, E is the electric field, B is the magnetic field (or magnetic induction if you prefer), and the integration is implicitly over all the volume of the system. The quantum mechanical, Heisenberg representation field operator for the radiation field is

$$\vec{A}_{\rm op}=\sum_{\vec{k}\vec{\lambda}}\left[A_{\vec{k}\vec{\lambda}}\vec{\lambda}\frac{e^{i(\vec{k}\cdot\vec{r}-\omega t)}}{\sqrt{V}}+\text{H.C.}\right]\ ,$$

where we have assumed box quantization with periodic boundary conditions, V is the volume of the box, and "H.C." stands for Hermitian conjugate. What is the time-averaged

Heisenberg representation of the Hamiltonian of the electromagnetic field $H_{\rm em}$ in terms of the operator $A^\dagger_{\vec k\vec\lambda}A_{\vec k\vec\lambda}$?

c) What is $H_{\rm em}$ in terms of dimensionless EM operators? What is the zero point energy of a radiation field: i.e., the energy expectation value for the state $|0,0,0,\ldots,0\rangle$?

d) Convert the summation for the zero point energy into an integral using the continuum approximation for the box quantization. What is the energy density $\mathcal{E}_0/V$ of the vacuum up to the mode with photon energy ϵ? (Note that ϵ is not the energy in the mode, it is the energy of photons in the mode: each photon has $\epsilon = \hbar\omega$.) What unfortunate thing happens if you set $\epsilon = \infty$?

---

024 qfull 00800 2 5 0 moderate thinking: commutation field operators

Extra keywords: (Ba-299:4)

4. The quantum mechanical, Heisenberg representation field operator for the radiation field is

$$\vec A_{\rm op}(\vec r,t) = \sum_{\vec k\vec\lambda}\left[A_{\vec k\vec\lambda}\vec\lambda\frac{e^{i(\vec k\cdot\vec r-\omega t)}}{\sqrt{V}} + \text{H.C.}\right] ,$$

where we have assumed box quantization with periodic boundary conditions, V is the volume of the box, and "H.C." stands for Hermitian conjugate.

a) Determine expressions for $\vec E_{\rm op}(\vec r,t)$ and $\vec B_{\rm op}(\vec r,t)$.

b) Determine $[\vec E_{\rm op}(\vec r,t),\vec B_{\rm op}(\vec r,t)]$. What can you say about the simultaneous knowledge that one can have about $\vec E$ and $\vec B$? **HINTS:** The following commutator relations will help simplify:

$$[A_{\vec k\vec\lambda},A_{\vec k'\vec\lambda'}]=0\ ,\qquad [A^\dagger_{\vec k\vec\lambda},A^\dagger_{\vec k'\vec\lambda'}]=0\ ,\qquad\text{and}\qquad [A_{\vec k\vec\lambda},A^\dagger_{\vec k'\vec\lambda'}]=\delta_{\vec k\vec k'}\delta_{\vec\lambda\vec\lambda'}\frac{2\pi\hbar c^2}{\omega}\ ,$$

where $\omega = kc$, of course. You will also have to deal with the outer product of two vectors which is a tensor: e.g., $\vec a\otimes\vec b$. The outer product is commutative: e.g., $\vec a\otimes\vec b = \vec b\otimes\vec a$ (e.g., ABS-25).

---

024 qfull 01500 2 5 0 moderate thinking: free particles non-radiate

Extra keywords: Reference Ba-280

5. Say you have a free particle (i.e., a free matter particle) in a momentum eigenstate with eigen momentum $\hbar\vec q_n$. Remember a free particle in the conventional sense of quantum mechanics means one not affected by any potentials at all. Using Fermi's golden rule you can try to calculate the particle's spontaneous emission when making a transition to another momentum eigen state with eigen momentum $\vec q_0$ (Ba-279). You find a momentum conservation rule is imposed:

$$\hbar\vec k = \hbar\vec q_n - \hbar\vec q_0\ ,$$

where $\hbar\vec k$ is the momentum of the emitted photon. But since you used the golden rule you also imposed energy conservation:

$$\hbar ck = \frac{\hbar^2 q_n^2}{2m} - \frac{\hbar^2 q_0^2}{2m}\ ,$$

where m is the particle's mass. The conclusion that is implied by these two relations is that free particles can't radiate at least not through the golden rule process used in the calculations. Show how the conclusion is reached. **HINT:** The two relations actually can be mutually satisfied in a mathematical sense: think about the assumptions implicit in them.

---

024 qfull 02000 3 5 0 moderate thinking: hydrogen spontaneous emission
Extra keywords: (Ba-300:7)

6. Consider a hydrogen atom with the nucleus fixed in space.

   a) What are all the states of the two lowest principal quantum numbers in spectroscopic notation: e.g., 2s($m = 0$) for n=2, ℓ=0 (which is what the s symbol means), and $m = 0$. Don't distinguish states by spin state.

   b) Between which states are there (electric dipole) allowed transitions transitions.

   c) The spontaneous emission power per solid angle in polarization $\vec{\lambda}$ in the electric dipole approximation is

   $$\frac{dP_\lambda}{d\Omega} = \frac{\omega^4 e^2}{2\pi c^3}|\vec{d}_{0n} \cdot \vec{\lambda}^*|^2 ,$$

   where

   $$\vec{d}_{0n} = \langle 0|\vec{R}|n\rangle$$

   is the dipole moment matrix element, $|n\rangle$ and $|0\rangle$ are, respectively, the initial and final states, and

   $$\vec{R} = \sum_i r_i$$

   is the position operator for all the particles in the system (Ba-282). Find the expression for $\vec{d}_{0n}$ between the 1s($m = 0$) and 2p($m = 0$) levels of hydrogen.

---

024 qfull 02500 2 5 0 moderate thinking: Einstein A coefficient
Extra keywords: See Ba-282, Gr-311–313

7. In the electric dipole approximation, the power in polarization λ per unit solid angle per particle (or system of particles) of a spontaneous transition process is

   $$\frac{dP_\lambda}{d\Omega} = \frac{\omega^4 e^2}{2\pi c^3}|\vec{d}_{0n} \cdot \vec{\lambda}^*|^2 ,$$

   where e is the charge on the particle (or particles),

   $$\vec{d}_{0n} = \langle 0|\vec{R}|n\rangle$$

   is the off-diagonal element of the dipole moment operator, and n and 0 label the initial and final states, respectively (Ba-282). In general,

   $$\vec{R} = \sum_i \vec{r}_i .$$

   where the sum is over the position operators of the particles in the system.

   a) Consider an ordinary 3-d Cartesian set of axes and radiation emitted along the z-axis. Consider the polarization vectors to be unit vectors in the x and y directions. The dipole matrix element points in an arbitrary direction (θ, ϕ) in spherical polar coordinates. What is the expression for power **SUMMED** over the two polarization directions in terms of the angle coordinates of the dipole matrix element? **HINTS:** A diagram probably helps and knowing how to express $\vec{d}_{0n}$ along Cartesian coordinates, but in spherical polar coordinates.

   b) Using the expression from the part (a) answer, find the total power radiated by integrating over all solid angle. **HINT:** Nothing forbids you from mentally transposing the z-axis from the general direction to a convenient direction.

c) What is the total photon number rate emitted from the transition (i.e., the Einstein A coefficient at least as Gr-312 defines it)?

d) If at time zero you have set of N_0 atoms in an excited state with only one downward transition available with Einstein A coefficient A and spontaneous emission as the only process, what is the population N at any time $t > 0$?

Chapt. 25 Second Quantization

Multiple-Choice Problems

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025 qmult 00100 1 1 2 easy memory: 2nd quantization

1. The formalism for quantizing fields is called:

    a) first quantization.
    b) second quantization.
    c) third quantization.
    d) fourth quantization.
    e) many quantization.

---

025 qmult 00200 1 4 3 easy deducto-memory: CA anti/commutation

2. "Let's play *Jeopardy*! For \$100, the answer is: These operators for a single mode have commutation relation $[a, a^\dagger] = 1$ for bosons and anticommutation relation $\{a, a^\dagger\} = 1$ for fermions."

    a) What are Hermitian operators, Alex?
    b) What are anti-Hermitian operators, Alex?
    c) What are creation and annihilation operators, Alex?
    d) What are penultimate and antepenultimate operators, Alex?
    e) What are genesis and revelations operators, Alex?

---

025 qmult 00300 1 1 1 easy memory: boson CA operator effects

3. For bosons the operators a and $a^\dagger$ acting on a state $|n\rangle$ give, respectively:

    a) $\sqrt{n}|n-1\rangle$ (or the null vector if $n=0$) and $\sqrt{n+1}|n\rangle$.
    b) $\sqrt{n-1}|n-1\rangle$ (or the null vector if $n=0$) and $\sqrt{n}|n\rangle$.
    c) $\sqrt{n}|-n+1\rangle$ (or the null vector if $n=0$) and $\sqrt{-n}|-n+1\rangle$.
    d) the null vector and the infinite vector.
    e) a non-vector and a non-non-vector.

---

025 qmult 00400 1 1 4 easy memory: fermion number operator

4. What are the eigenvalues of the fermion number operator obtained from the matrix representation this operator: i.e., from

$$N = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} ?$$

    a) ±1
    b) Both are zero.
    c) 1 and 2.
    d) 0 and 1.
    e) ±2.

---

025 qmult 00500 1 1 1 easy memory: number operators commute

5. The number operators for different modes for the boson and fermion cases:

   a) commute.
   b) anticommute
   c) commute and anticommute, respectively.
   d) anticommute and commute, respectively.
   e) promote and demote, respectively.

---

025 qmult 00600 1 1 2 easy memory: CA operators for symmetrization

6. Symmetrized states in second quantization formalism are easily constructed using

   a) annihilation operators.
   b) creation operators.
   c) more annihilation operators than creation operators.
   d) steady-state operators.
   e) degenerate operators.

---

025 qmult 00700 1 4 5 easy deducto-memory: field operators

7. "Let's play *Jeopardy*! For \$100, the answer is: These operators are constructed from the creation and annihilation operators in second quantization formalism."

   a) What are the copse operators, Alex?
   b) What are the glade operators, Alex?
   c) What are the meadow operators, Alex?
   d) What are the field marshal operators, Alex?
   e) What are the field operators, Alex?

---

025 qmult 01000 1 4 4 easy deducto-memory: 2nd QM density operator

Extra keywords: Reference Ba-422

8. "Let's play *Jeopardy*! For \$100, the answer is:

$$\rho(\vec{r}\,) = \Psi_s(\vec{r}\,)^\dagger \Psi_s(\vec{r}\,) ,$$

where $\Psi_s(\vec{r}\,)^\dagger$ and $\Psi_s(\vec{r}\,)$ are the field creation and annihilation operators at a point $\vec{r}$ with spin coordinate s."

   a) What is a non-Hermitian operator, Alex?
   b) What is the density expectation value, Alex?
   c) What is the first quantization density operaty, Alex?
   d) What is the second quantization particle density operator, Alex?
   e) What is it's Greek to me, Alex?

---

025 qmult 01010 1 1 1 easy memory: density operator expectation value

Extra keywords: See Ba-422

9. There is a second quantization operator

$$\rho(\vec{r}\,) = \Psi_s(\vec{r})^\dagger \Psi_s(\vec{r}\,) ,$$

where $\Psi_s(\vec{r}\,)^\dagger$ and $\Psi_s(\vec{r}\,)$ are the field creation and annihilation operators at a point $\vec{r}$ with spin coordinate s. Its expectation value is:

   a) the mean density of particles per unit volume.
   b) the normalization constant of the state $|\Phi\rangle$ *IT* is applied to.
   c) the pair correlation function.

d) the pair anti-correlation function.
e) the one-particle density matrix.

---

025 qmult 01100 1 1 3 easy memory: zeros of one-particle density matrix
Extra keywords: See Ba-426

10. The one-particle density matrix for non-interacting, spin 1/2 fermions in the ground state of a box quantization system is

$$G_s(\vec{r}-\vec{r}\,') = \frac{3n}{2}\frac{\sin(x)-x\cos(x)}{x^3} \ ,$$

where n is the expectation particle density of the ground state and $x = p_{\rm f}|\vec{r}-\vec{r}\,'|$ (i.e., Fermi momentum times displacement vector). The zeros of this function are approximately given by:

a) $x = n$, where $n = 0, 1, 2, \ldots$
b) $x = n\pi$, where $n = 1, 2, 3, \ldots$
c) $x = (1/2 + n)\pi$, where $n = 1, 2, 3, \ldots$
d) $x = (1/2 + n)\pi$, where $n = 0, 1, 2, \ldots$
e) $x = n\pi$, where $n = 0, 1, 2, \ldots$

---

025 qmult 01300 1 1 2 easy memory: pair correlation function
Extra keywords: See Ba-429

11. For a box quantization system of non-interacting, spin 1/2 fermions in the ground state we have the useful function

$$g_{ss'}(\vec{r}-\vec{r}\,') = \begin{cases} 1 & \text{for } s \neq s'; \\ 1 - \dfrac{9}{x^6}[\sin(x)-x\cos(x)]^2 & \text{for } s = s'. \end{cases}$$

where and $x = p_{\rm f}|\vec{r}-\vec{r}\,'|$ (i.e., Fermi momentum times displacement vector). This function is the:

a) pair anti-correlation function.
b) pair correlation function.
c) pair annihilation function.
d) pair creation function.
e) one-particle density matrix.

---

025 qmult 01700 1 4 3 easy deducto-memory: exchange effect

12. "Let's play *Jeopardy*! For \$100, the answer is: This effect generally decreases the absolute value of the potential energy of an interaction between fermions of the same spin coordinate—except in the unusual case that the interaction increases with **INCREASING** distance between the fermions."

a) What is expunge effect, Alex?
b) What is the interchange effect, Alex?
c) What is the exchange effect, Alex?
d) What is the interstate effect, Alex?
e) What is the exchange rate effect, Alex?

---

025 qmult 02000 1 1 2 easy memory: Feynman diagrams
Extra keywords: See Ha-211

13. As a visualization of the terms in an interaction perturbation series in second quantization formalism, one can use:

a) Feynman landscapes.

b) Feynman diagrams.
c) Feynman water colors.
d) Feynman lithographs.
e) Feynman doodles.

Full-Answer Problems

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025 qfull 00100 2 5 0 moderate thinking: boson CA proofs

1. Let's do proofs with the boson creation and annihilation (CA) operators a and $a^\dagger$ for a single mode. Recall $[a, a^\dagger] = 1$ is their fundamental commutation relation.

   a) The number operator is defined by $N = a^\dagger a$. Show that N is Hermitian. Assume N is an observable (i.e., a Hermitian operator with a complete set of eigenstates for whatever space we are dealing with) and let its eigen-equation be

   $$N|n\rangle = n|n\rangle \ .$$

   We also assume there is no degeneracy. Show that $n \geq 0$ and that $a|0\rangle = 0$ (i.e., $a|0\rangle$ is the null vector). **HINT:** Make use of the rule—which I think is valid—at least lots of sources use it or so I seem to recall—that a legitimate operator acting on a vector always yields a vector.

   b) Find explicit expressions for $[N, a]$ and $[N, a^\dagger]$.

   c) Show that $a^\dagger|n\rangle$ and $a|n\rangle$ are eigenstates of N and find explicit expressions for them.

   d) Show that n must be an integer.

   e) Find a general expression for $|n\rangle$ in terms of the vacuum state $|0\rangle$. Make sure that $|n\rangle$ is properly normalized.

   f) Since the $|n\rangle$ are non-degenerate states of the number operator $N = a^\dagger a$ (an observable), they are guaranteed to be orthogonal. But for the sake of paranoia vis-à-vis the universe, show explicitly that

   $$\langle m|n\rangle = \delta_{mn} \ ,$$

   making use of the part (e) answer and assuming the vacuum state is properly normalized. **HINT:** This is easy after you've seen the trick.

   g) Prove $[a, (a^\dagger)^n] = n(a^\dagger)^{n-1}$ for $n \geq 1$.

---

025 qfull 00200 2 5 0 moderate thinking: 2 mode fermion CA operators

Extra keywords: (Ba-439:1)

2. Let us consider the two-mode fermion case.

   a) Construct explicit 4×4 matrix representations of the creation and annihilation (CA) operators a_0, $a_0^\dagger$, a_1, and $a_2^\dagger$. **HINT:** See Ba-414–415.

   b) Construct explicit 4×4 matrix representations of the number operators N_0, N_1, and $N = N_0 + N_1$. What are the eigenvalues and eigenvectors the of number operators? Are there any degeneracies?

   c) Confirm that the all commutation relations given on Ba-416 hold for the CA operators in the matrix representation. **HINT:** I gave up after doing

   $$\{a_0, a_0^\dagger\} = 1 \qquad \text{and} \qquad \{a_0, a_1^\dagger\} = 0 \ .$$

---

025 qfull 00300 2 5 0 moderate thinking: one-particle density matrix

Extra keywords: See Ba-425

3. A quantity that turns out to be useful in studying non-interacting, spin 1/2 fermions in a box quantization system of volume V is the one-particle density matrix defined by

$$G_s(\vec{r}-\vec{r}\,') = \langle\Phi_0|\Psi_s(\vec{r})^\dagger\Psi_s(\vec{r}\,')|\Phi_0\rangle \ ,$$

where $|\Phi_0\rangle$ is the ground state and

$$\Psi_s(\vec{r})^\dagger = \sum_{\vec{p}} \frac{e^{-i\vec{p}\cdot\vec{r}}}{\sqrt{V}} a^\dagger_{\vec{p}s} \qquad \text{and} \qquad \Psi_s(\vec{r}) = \sum_{\vec{p}} \frac{e^{i\vec{p}\cdot\vec{r}}}{\sqrt{V}} a_{\vec{p}s}$$

are the field creation and annihilation operators with $\hbar$ set to 1 and where s is the z-quantum number for the spin state. Recall that the ground state has all the states occupied for $|\vec{p}| \leq p_{\rm f}$, where $p_{\rm f}$ is the Fermi momentum. to

a) Find an expression for $G_s(0)$ using the approximation of a continuum of states. What, in fact, is this quantity?

b) Show that $G_s(\vec{r}-\vec{r}\,')$ is given by

$$G_s(\vec{r}-\vec{r}\,') = \frac{3n}{2}\frac{\sin(x) - x\cos(x)}{x^3} \ ,$$

where $x \equiv p_{\rm f}|\vec{r}-\vec{r}\,'|$, n is the mean density, and the approximation of a continuum of states has been used. **HINT:** The integrand is not isotropic in this case, but one can choose the z-axis for maximum simplicity.

c) Now let us analyze the dimensionless $G_s(\vec{r}-\vec{r}\,')$ given by

$$g(x) = \frac{\sin(x) - x\cos(x)}{x^3} \ ,$$

where only x greater than is meaningful, of course. First, what is the variation in x usually to be thought to be attributed to? Second, what are the small x and large x limiting forms of $g(x)$: give the small x limiting form to 4th order in x. Third, give an approximate expression for the zeros of $g(x)$. Fourth, sketch $g(x)$.

d) Now find a convergent iteration formula that allows you to solve for the zeros of $g(x)$. Implement this formula in a computer code and compute the first ten zeros to good accuracy.

---

025 qfull 00400 2 5 0 moderate thinking: fermion pair correlation

Extra keywords: See Ba-428–429 and Ar-527

4. The pair correlation function for spin 1/2 fermions in the ground state of a box quantization system is

$$g_{ss'}(\vec{r}-\vec{r}\,') = \begin{cases} 1 \ , & \text{for } s \neq s'; \\ 1 - \dfrac{9}{x^6}[\sin(x) - x\cos(x)]^2 \ , & \text{for } s = s', \end{cases}$$

where s is a spin coordinate label, $x = p_{\rm f}|\vec{r}-\vec{r}\,'|$, $p_{\rm f}$ is the Fermi momentum, $\vec{r}$ is the point where a fermion has be removed, and $\vec{r}\,'$ is the point where one has measured the particle density just after the removal of the fermion (Ba-428–429). The expectation particle density density for a given is spin coordinate is $(n/2)g_{ss'}(\vec{r}-\vec{r}\,')$, where $n = N/V$ is the original expectation density of a spin state: N is the number of particles in the system and V is the system volume.

a) Prove that $(n/2)g_{ss'}(\vec r-\vec r\,')$ is properly scaled for $s\neq s'$: i.e., that the integral of $(n/2)g_{ss'}(\vec r-\vec r\,')$ over all volume is the right number of particles.

b) Now prove that $(n/2)g_{ss'}(\vec r-\vec r\,')$ is properly scaled for $s=s'$. **HINT:** You might have to look up the properties of the spherical Bessel functions—unless you know those like the back of your hand.

---

025 qfull 00450 2 5 0 moderate thinking: 2nd quantization potential

Extra keywords: See Ba-434

5. The 2nd quantization operator for a two-body potential $V(\vec r-\vec r\,')$ between identical particles is

$$V_{\rm 2nd}=\frac{1}{2}\sum_{s's}\int d\vec r\,'\,d\vec r\,V(\vec r-\vec r\,')\Psi_s(\vec r)^\dagger\Psi_{s'}(\vec r\,')^\dagger\Psi_{s'}(\vec r\,')\Psi_s(\vec r)\ ,$$

where the 1/2 prevents double counting in the integration, the sum is over all spin states, and the $\Psi^\dagger$'s and Ψ's are the field creation and annihilation operators. Prove that $V_{\rm 2nd}$ is correct by showing that a matrix element of $V_{\rm 2nd}$ with general, properly symmetrized, n particle states $|\Phi'\rangle$ and $|\Phi\rangle$ (i.e., $\langle\Phi'|V_{\rm 2nd}|\Phi\rangle$) is the same as the matrix element of the same states with the 1st quantization operator for n identical particles: i.e.,

$$V_{\rm 1st}=\frac{1}{2}\sum_{ij,i\neq j}V(\vec r_i-\vec r_j)\ ,$$

where the 1/2 prevents double counting. **HINTS:** You should recall the effect of a field creation operator on a localized state of $n-1$ particles: i.e.,

$$\Psi_s(\vec r)^\dagger|\vec r_1s_1,\ldots,\vec r_{n-1}s_{n-1}\rangle=\sqrt{n}|\vec r_1s_1,\ldots,r_{n-1}s_{n-1},r_ns_n\rangle$$

(Ba-419) Also recall localized state unit operator for a properly symmetrized states of n particles is

$$\mathbf{1}_n=\sum_{s_1\ldots s_n}\int d\vec r_1\ldots\vec r_n\,|\vec r_1s_1,\ldots,\vec r_ns_n\rangle\langle\vec r_1s_1,\ldots,\vec r_ns_n|$$

(Ba-421).

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025 qfull 00500 3 5 0 tough thinking: fermion Coulomb exchange

Extra keywords: See Ba-436

6. The exchange energy per electron for a ground state electron gas is given by

$$\frac{E}{N}=-\frac{9\pi ne^2}{p_{\rm f}^2}\int_0^\infty\frac{[\sin(x)-x\cos(x)]^2}{x^5}\,dx\ ,$$

where N is electron number, n is electron density, $p_{\rm f}$ is the Fermi momentum, and $x=p_{\rm f}r$ is a dimensionless radius for an integration over all space (Ba-436).

a) First, let us analyze the integrand of the integral. Where are its zeros approximately for $x\geq 0$? What is its small x behavior to 5th order in small x? What is its large x behavior? Sketch the integrand.

b) Now evaluate the integral approximately or exactly by analytic means. **HINT:** An exact analytic integration must be possible, but probably one must use some special method. For approximate analytic integration, just do the best you can.

c) Now evaluate the integral numerically to high accuracy. **HINT:** Simpson's rule with double precision fortran works pretty well.

---

025 qfull 00600 2 5 0 moderate thinking: two fermions in a box

Extra keywords: (Ba-439:4)

7. Consider a box quantization system with volume V: the single-particle eigenstates recall are given by

$$\phi_s(\vec{r}\,) = \frac{e^{i\vec{p}\cdot\vec{r}}}{V} \ ,$$

where periodic boundary conditions have been imposed, $\hbar$ has been set to 1, and s gives the spin coordinate. We will consider two spin 1/2 fermions in the box in state

$$|1_{\vec{p}_1 s_1}, 1_{\vec{p}_2 s_2}\rangle = a^\dagger_{\vec{p}_2 s_2} a^\dagger_{\vec{p}_1 s_1}|0\rangle \ ,$$

where the $a^\dagger$'s are creation operators and $|0\rangle$ is the vacuum state (Ba-417). Recall the anticommutation relations for the fermion creation and annihilation operators:

$$\{a_{\vec{p}s}, a^\dagger_{\vec{p}'s'}\} = \delta_{\vec{p}\vec{p}'}\delta_{ss'} \ , \qquad \{a_{\vec{p}s}, a_{\vec{p}'s'}\} = 0 \ , \qquad \text{and} \qquad \{a^\dagger_{\vec{p}s}, a^\dagger_{\vec{p}'s'}\} = 0 \ ,$$

where the $a^\dagger$'s are again creation operators and the a's are annihilation operators (Ba-417).

a) Show that

$$\langle 1_{\vec{p}_1 s_1}, 1_{\vec{p}_2 s_2}|1_{\vec{p}_1 s_1}, 1_{\vec{p}_2 s_2}\rangle = 1 - \delta_{\vec{p}_1\vec{p}_2}\delta_{s_1 s_2} \ .$$

What is the interpretation of this result?

b) You are now given the operator

$$a^\dagger_{\vec{p}s} a^\dagger_{\vec{q}s'} a_{\vec{q}\,'s'} a_{\vec{p}\,'s} \ .$$

Write out the explicit expectation value of the operator for the $|1_{\vec{p}_1 s_1}, 1_{\vec{p}_2 s_2}\rangle$ state. **HINTS:** Remember to make use of the annihilation property $a|0\rangle = 0$. There are a lot of tedious Kronecker deltas.

c) One form of the 2nd quantization two-body interaction operator is

$$v_{\text{2nd}} = \frac{1}{2}\frac{1}{V^2}\sum_{pp'qq'}\sum_{ss'}\int d\vec{r}\,d\vec{r}\,'\,v(\vec{r}-\vec{r}\,')e^{-i(\vec{p}-\vec{p}\,')\cdot\vec{r}}e^{-i(\vec{q}-\vec{q}\,')\cdot\vec{r}\,'}\,a^\dagger_{\vec{p}s} a^\dagger_{\vec{q}s'} a_{\vec{q}\,'s'} a_{\vec{p}\,'s} \ ,$$

where V again is volume, $v(\vec{r}-\vec{r}\,')$ is the two-body potential function, and $a^\dagger_{\vec{p}s} a^\dagger_{\vec{q}s'} a_{\vec{q}\,'s'} a_{\vec{p}\,'s}$ is the operator from the part (b) question. Making use of the part (b) answer express expectation value $\langle 1_{\vec{p}_1 s_1}, 1_{\vec{p}_2 s_2}|v_{\text{2nd}}|1_{\vec{p}_1 s_1}, 1_{\vec{p}_2 s_2}\rangle$ as simply as possible. Don't assume that surface effects can be neglected. What is the use or significance of this matrix element? **HINTS:** The summations allow one to kill most of the Kroneckar deltas and get a pretty simple expression, but the explicit integrations are still there.

d) Say the two fermions are in different spin states and the two-body potential $v(\vec{r}-\vec{r}\,') = C$, where C is a constant. What is the expectation value from the part (c) answer in this case?

Chapt. 26 Klein-Gordon Equation

Multiple-Choice Problems

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026 qmult 00100 1 4 4 easy deducto-memory: Klein-Gordan eqn

Extra keywords: See the biography of Schrodinger and BJ-343

1. "Let's play *Jeopardy*! For \$100, the answer is: A relativistic quantum mechanical particle equation originally invented by Schrödinger (but never published by him) whose valid interpretation was provided by Pauli and Weisskopf."

   a) What is the 2nd Schrödinger equation, Alex?
   b) What is the relativistic Schödinger equation, Alex?
   c) What is the Pauli-Weisskopf equation, Alex?
   d) What is the Klein-Gordon equation, Alex?
   e) What is the small Scotsman equation, Alex?

---

026 qmult 00200 2 1 2 moderate memory: KG eqn development

Extra keywords: See Ba-501

2. To develop the free-particle Klein-Gordon equation one assumes that the operators $E_{\rm op} = i\hbar\partial/\partial t$ and $p_{\rm op} = (\hbar/i)\nabla$ apply in relativistic quantum mechanics and then applies the correspondence principle to the non-quantum-mechanical special relativity result:

   a) $E = \sqrt{(pc)^2 + (mc^2)^2}$.
   b) $E^2 = (pc)^2 + (mc^2)^2$.
   c) $\gamma = 1/\sqrt{1-\beta^2}$.
   d) $E = mc^2$.
   e) $\ell = \ell_{\rm proper}\sqrt{1-\beta^2}$.

---

026 qmult 00300 1 1 2 easy memory: antiparticles

Extra keywords: See Ba-506

3. The free-particle Klein-Gordon equation leads to two energy eigen-solutions for each momentum eigenvalue. The two energies are equal in absolute value and opposite in sign in one interpretation. The negative energy solution can, in fact, be interpreted as a positive energy solution for:

   a) a helium atom.
   b) an antiparticle.
   c) a wavicle.
   d) an anti-wavicle.
   e) an anti-wastrel.

---

026 qmult 00400 1 1 4 easy memory: KG density and current density

Extra keywords: See Ba-503 and BJ-343

4. The density and current density that one obtains from the Klein-Gordon wave function are interpreted, respectively, as:

   a) anti-density and anti-current density.

b) improbability density and current density.
c) current density and density in a relativistic reversal.
d) expectation value charge density and charge current density.
e) probability density and probability current density.

Full-Answer Problems

026 qfull 00300 2 5 0 moderate thinking: Lorentz transf. of KG eqn

Extra keywords: See Ba-502

1. One form of the free-particle Klein-Gordon (KG) equation is

$$K_{\rm op}\Psi(\vec{r},t)=\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2}-\nabla^2+\left(\frac{mc}{\hbar}\right)^2\right]\Psi(\vec{r},t)=0\ ,$$

where $K_{\rm op}$ is here just an abbreviation for the Klein-Gordon equation operator and m is rest mass (Ba-501). This equation is supposed to be relativistically correct. This means that it must be the correct physics to apply to the particle in any inertial frame. But how does the solution $\Psi(\vec{r},t)$ change on transformation from one inertial frame to another?

To find out, consider the special case of a transformation between frames S and S', where the S' is moving at velocity β (in units of c) along the mutual x-axis of the two frames. The origins of the two frames were coincident at $\tau=\tau'=0$ (where $\tau=ct$: i.e., time in units of distance). The special Lorentz transformations in this case are

$$x'=\gamma(x-\beta\tau)\ ,\qquad \tau'=\gamma(\tau-\beta x)\ ,\qquad y'=y\ ,\qquad\text{and}\qquad z'=z\ ,$$

where the Lorentz factor

$$\gamma=\frac{1}{\sqrt{1-\beta^2}}\ .$$

Now transform $K_{\rm op}\Psi(\vec{r},t)=0$ to the primed system (i.e., write it terms of the $\vec{r}\,'$ and t' variables). Does the transformed equation $K'_{\rm op}\Psi[\vec{r}=f(\vec{r}\,',t'),t=f(\vec{r}\,',t')]=0$ have the same form as the untransformed equation: i.e., does it look like

$$\left[\frac{1}{c^2}\frac{\partial^2}{\partial t'^2}-\nabla'^2+\left(\frac{mc}{\hbar}\right)^2\right]\Psi(\vec{r}\,',t')'=0$$

when $\Psi[\vec{r}=f(\vec{r}\,',t'),t=f(\vec{r}\,',t')]$ is identified as $\Psi(\vec{r}\,',t')'$? What kind of object is $\Psi(\vec{r},t)$: i.e., scalar, vector, tensor? **HINT:** Recall the chain rule.

Multiple-Choice Problems

Full-Answer Problems

030 qfull 00100 2 5 0 moderate thinking: eph Bose-Einstein condensate

Extra keywords: Greiner et al. 2002, 415, 39 with Stoof review on p. 25

1. Go to the library 2nd floor reading room and find the 20002jan03 issue of *Nature* (it may have been placed under the display shelf) and read the commentary article by Stoof on page 25 about a quantum phase transition from a Bose-Einstein condensate to a Mott insulator. What do you think Stoof really means when he says in the superfluid state "atoms still move freely from one valley to the next"? **NOTE:** The instructor disavows any ability to completely elucidate this commentary or the research article by Greiner et al. it comments on.

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030 qfull 00200 2 3 0 moderate thinking: eph quantum gravity well

Extra keywords: reference: Nesvizhevsky et al. 2002, Nature, 413, 297

2. Is the gravity subject to quantum mechanical laws or is it somehow totally decoupled? Everyone really assumes that gravity is subject to quantum mechanical laws, but the assumption is not well verified experimentally: in fact it may never have been verified at all until now—not that I would know. The lack of experimental verification is because gravity is so infernally weak compared to other forces in microscopic experiments that it is usually completely negligible. Recently Nesviszhevsky et al. (2002, Nature, 413, 297) have reported from an experiment that a gravity well (at least part of the constraining potential is gravitational) does have quantized energy states. This appears to be the first time that such an experimental result has been achieved. It's a wonderful result. Of course, if they hadn't found quantization, it would have been a shock and most people would have concluded that the experiment was wrong somehow. Experiment may be the ultimate judge of theory, but experiment can certainly tell fibs for awhile.

   Go read Nesviszhevsky et al. in the 2nd floor reading room of the library: the relevant issue may be under the shelf. If a neutron in the theoretically predicted gravity well made a transition from the 1st excited state to the ground state and emitted a photon, what would be the wavelength of the photon? Could such a photon be measured? What classically does such a transition correspond to?

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030 qfull 00300 1 5 0 easy thinking: eph quantum computing

Extra keywords: Reference Seife, C. 2001, Science, 293, 2026

3. Read the article on quantum computing by Seife (2001, Science, 293, 2026) and make an estimate of how long it will be before for there is a quantum computer that solves a computational problem not solvable by a classical computer: I'm excepting, of course, any problems concerning quantum computer operation itself. Give your reasoning. All answers are right—and wrong—or in a superposition of those two states. My answer is 1 year. **HINT:** You can probably find the issue in the library, but there's one in the physics lounge near the Britney issue. Primers on quantum computing can be found by going to

   http://www.physics.unlv.edu/~jeffery/images/science

   and clicking down through quantum mechanics and quantum computing.

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030 qfull 00400 2 5 0 moderate thinking: eph C-70 diffraction

Extra keywords: Reference Nairz et al. 2001, quant-ph/0105061

4. On the web go to the Los Alamos eprint archive:

   http://xxx.lanl.gov/ .

   There click on search and then on search for articles by Zeilinger under the quant-ph topic. Locate Nairz, Arndt, & Zeilinger 2001, quant-ph/0105061 and download it. This is article reports the particle diffraction for C_{70} (a fullerene). There should be great pictures on the web of fullerenes, but the best I could find were at

   http://www.sussex.ac.uk/Users/kroto/fullgallery.html

   and

   http://cnst.rice.edu/pics.html

and these don't have descriptions. Fullerenes are the largest particles ever shown to diffract: their size scale must be order-of a nanometer: 10 times ordinary atomic size. The article calls itself a verification of the Heisenberg uncertainty principle. In a general sense this is absolutely true since they verify the wave nature of particle propagation. But it isn't a direct test of the formal uncertainty relation

$$\sigma_x \sigma_{p_x} \geq \frac{\hbar}{2} ,$$

where σ_x and σ_{p_x} are standard deviations of x-direction position and momentum, respectively, for the wave function (e.g., Gr-18, Gr-108–110). Explain why it isn't a direct test. **HINTS:** You should all have studied physical optics at some point. Essentially what formula are they testing?

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030 qfull 00500 1 5 0 easy thinking: bulk and branes

Extra keywords: Reference Arkani-Hamed, N., et al. 2002, Physics Today, February, 35

5. Go the library basement and read the article by Arkani-Hamed et al. (Physics Today, February, p. 35). Perhaps a 2nd reading would help or a course in particle physics. Anyway what is the bulk (not Hulk, bulk) and the brane (not Brain, brane)?

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030 qfull 00600 1 5 0 easy thinking: sympathetic cooling

Extra keywords: O'Hara & Thomas, 2001, Science, March 30, 291, 2556

6. Go to the library or the physics lounge and read O'Hara & Thomas (2001, Science, March 30, 291, p. 2556) on degenerate gases of bosons and fermions. What is sympathetic cooling?

Appendix 1 Mathematical Problems

Multiple-Choice Problems

Full-Answer Problems

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031 qfull 00100 2 3 0 moderate math: Gauss summations

1. Gauss at the age of two proved various useful summation formulae. Now we can do this too maybe.

   a) Prove

   $$S_0(n) = \sum_{\ell=1}^{n} 1 = n \ .$$

   HINT: This is really very easy.

   b) Prove

   $$S_1(n) = \sum_{\ell=1}^{n} \ell = \frac{n(n+1)}{2} \ .$$

   HINT: The trick is to add to every term in the sum its "complement" and then sum those 2-sums and divide by 2 to account for double counting.

   c) Prove

   $$S_2(n) = \sum_{\ell=1}^{n} \ell^2 = \frac{n(n+1)(2n+1)}{6} \ .$$

   HINT: A proof by induction works, but for that proof you need to know the result first and that's the weak way. The stronger way is to reduce the problem to an already solved problem. Consider the general summation formula

   $$S_k(n) = \sum_{\ell=1}^{n} \ell^k \ .$$

   For each ℓ, you can construct a column of ℓ^{k-1}'s that is ℓ in height. Can you add up the values in the table that is made up of these columns in some way to get $S_k(n)$.

   d) Prove

   $$S_3(n) = \sum_{\ell=1}^{n} \ell^3 = \frac{n^2(n+1)^2}{4} \ .$$

   HINT: This formula can be proven using the "complement" trick and the formulae of parts (b) and (c). It can also more tediously be solved by the procedure hinted at in part (c). Or, of course, induction will work.

---

031 qfull 00200 1 3 0 easy math: uniqueness of power series

2. Power series are unique.

   a) Prove that coefficients a_k of the power series

   $$P(x) = \sum_{k=0}^{\infty} a_k x^k$$

   are unique choices given that the series is convergent of course. **HINT:** The mth derivative of $P(x)$ evaluated at $x = 0$ can have only one value.

   b) Prove that coefficients $a_{k\ell}$ of the double power series

   $$P(x, y) = \sum_{k=0,\ell=0}^{\infty,\infty} a_{k\ell} x^k y^\ell$$

   are unique choices given that the series is convergent of course. **HINT:** *Mutatis mutandis.*

---

031 qfull 00300 2 5 0 moderate thinking: Leibniz's formula (Ar-558) proof

3. Prove Leibniz's formula (Ar-558)

   $$\frac{d^n(fg)}{dx^n} = \sum_{k=0}^{n} \binom{n}{k} \frac{d^k f}{dx^k} \frac{d^{n-k} g}{dx^{n-k}}$$

   by induction.

---

031 qfull 00400 2 5 0 moderate thinking: integrals of type xe**-2

4. In evaluating anything that depends on a Gaussian distribution (e.g., the Maxwell-Boltzmann distribution of classical statistical mechanics), one frequently has to evaluate integrals of the type

   $$I_n = \int_0^\infty x^n e^{-\lambda x^2}\, dx \ ,$$

   where n is an odd positive integer.

   a) Solve for I_1.

   b) Obtaining the general formula for I_n is now trivial with a magic trick. Act on I_1 with the operator

   $$\left(-\frac{d}{d\lambda}\right)^{(n-1)/2} \quad .$$

   c) From the general formula evaluate I_1 I_3, I_5, and I_7.

---

031 qfull 01000 2 5 0 moderate thinking:

5. In understanding determinants some permutation results must be proven. The proofs are expected to be cogent and memorable rather than mathematical rigorous.

   a) Given n objects, prove that there are $n!$ permutations for ordering them in a line.

   b) If you interchange any two particles in a given permutation, you get another permutation. Let's call that action an exchange. If you exchange nearest nearest neighbors, let's call that a nearest neighbor or NN exchange. Prove that any exchange requires an odd number of NN exchanges.

c) Permutations have definite parity. This means that going from one definite permutation to another definite permutation by any possible series of NN exchanges (i.e., by any possible path) will always involve either an even number of NN exchanges or an odd number: i.e., if one path is even/odd, then any other path is even/odd. Given that definite parity is true prove that any path of NN exchanges from a permutation that brings you back to that permutation (i.e., a closed path) has an even number of NN exchanges.

d) Now we have to prove definite parity exists. Say there is a fiducial permutation which by definition we say has even parity. If definite parity exists, then every other permutation is definitely even or odd relative to the fiducial permutation. If $n = 1$, does definite parity hold in this trivial case? For $n \geq 2$, prove that definite parity holds. **HINTS:** It suffices to prove that going from the fiducial permutation to any other permutation always involves a definite even or odd path since the fiducial permutation is arbitrary. Proof by induction might be the best route. I can't see how brief word arguments can be avoided.

e) Now prove for $n \geq 2$ that there are an equal number of even and odd permutations. **HINT:** Consider starting with an even permutation and systematically by an NN exchange path going through all possible permutations. Then start with an odd permutation and follow the same NN exchange path.

Appendix 2 Quantum Mechanics Equation Sheet

Note: This equation sheet is intended for students writing tests or reviewing material. Therefore it neither intended to be complete nor completely explicit. There are fewer symbols than variables, and so some symbols must be used for different things.

---

1 Constants not to High Accuracy

Constant Name	Symbol	Derived from CODATA 1998
Bohr radius	$a_{\text{Bohr}} = \dfrac{\lambda_{\text{Compton}}}{2\pi\alpha}$	$= 0.529\,\text{Å}$
Boltzmann's constant	k	$= 0.8617 \times 10^{-6}\,\text{eV}\,\text{K}^{-1}$ $= 1.381 \times 10^{-16}\,\text{erg}\,\text{K}^{-1}$
Compton wavelength	$\lambda_{\text{Compton}} = \dfrac{h}{m_e c}$	$= 0.0246\,\text{Å}$
Electron rest energy	$m_e c^2$	$= 5.11 \times 10^5\,\text{eV}$
Elementary charge squared	e^2	$= 14.40\,\text{eV}\,\text{Å}$
Fine Structure constant	$\alpha = \dfrac{e^2}{\hbar c}$	$= 1/137.036$
Kinetic energy coefficient	$\dfrac{\hbar^2}{2m_e}$	$= 3.81\,\text{eV}\,\text{Å}^2$
	$\dfrac{\hbar^2}{m_e}$	$= 7.62\,\text{eV}\,\text{Å}^2$
Planck's constant	h	$= 4.15 \times 10^{-15}\,\text{eV}$
Planck's h-bar	$\hbar$	$= 6.58 \times 10^{-16}\,\text{eV}$
	hc	$= 12398.42\,\text{eV}\,\text{Å}$
	$\hbar c$	$= 1973.27\,\text{eV}\,\text{Å}$
Rydberg Energy	$E_{\text{Ryd}} = \dfrac{1}{2} m_e c^2 \alpha^2$	$= 13.606\,\text{eV}$

2 Some Useful Formulae

Leibniz's formula
$$\frac{d^n(fg)}{dx^n} = \sum_{k=0}^{n} \binom{n}{k} \frac{d^k f}{dx^k} \frac{d^{n-k} g}{dx^{n-k}}$$

Normalized Gaussian
$$P = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x - \langle x \rangle)^2}{2\sigma^2}\right]$$

3 Schrödinger's Equation

$$H\Psi(x,t) = \left[\frac{p^2}{2m} + V(x)\right]\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

$$H\psi(x) = \left[\frac{p^2}{2m} + V(x)\right]\psi(x) = E\psi(x)$$

$$H\Psi(\vec{r},t) = \left[\frac{p^2}{2m} + V(\vec{r})\right]\Psi(\vec{r},t) = i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} \qquad H|\Psi\rangle = i\hbar\frac{\partial}{\partial t}|\Psi\rangle$$

$$H\psi(\vec{r}) = \left[\frac{p^2}{2m} + V(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r}) \qquad H|\psi\rangle = E|\psi\rangle$$

---

4 Some Operators

$$p = \frac{\hbar}{i}\frac{\partial}{\partial x} \qquad p^2 = -\hbar^2\frac{\partial^2}{\partial x^2}$$

$$H = \frac{p^2}{2m} + V(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

$$p = \frac{\hbar}{i}\nabla \qquad p^2 = -\hbar^2\nabla^2$$

$$H = \frac{p^2}{2m} + V(\vec{r}) = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$$

$$\nabla = \hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y} + \hat{z}\frac{\partial}{\partial z} = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\theta}\frac{1}{r\sin\theta}\frac{\partial}{\partial \theta}$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

---

5 Kronecker Delta and Levi-Civita Symbol

$$\delta_{ij} = \begin{cases} 1, & i = j; \\ 0, & \text{otherwise} \end{cases} \qquad \varepsilon_{ijk} = \begin{cases} 1, & ijk \text{ cyclic;} \\ -1, & ijk \text{ anticyclic;} \\ 0, & \text{if two indices the same.} \end{cases}$$

$$\varepsilon_{ijk}\varepsilon_{i\ell m} = \delta_{j\ell}\delta_{km} - \delta_{jm}\delta_{k\ell} \qquad \text{(Einstein summation on } i\text{)}$$

---

6 Time Evolution Formulae

$$\text{General} \qquad \frac{d\langle A\rangle}{dt} = \left\langle\frac{\partial A}{\partial t}\right\rangle + \frac{1}{\hbar}\langle i[H(t), A]\rangle$$

$$\text{Ehrenfest's Theorem} \qquad \frac{d\langle\vec{r}\rangle}{dt} = \frac{1}{m}\langle\vec{p}\rangle \qquad \text{and} \qquad \frac{d\langle\vec{p}\rangle}{dt} = -\langle\nabla V(\vec{r})\rangle$$

$$|\Psi(t)\rangle = \sum_j c_j(0)e^{-iE_jt/\hbar}|\phi_j\rangle$$

---

7 Simple Harmonic Oscillator (SHO) Formulae

$$V(x) = \frac{1}{2}m\omega^2x^2 \qquad \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2x^2\right)\psi = E\psi$$

$$\beta = \sqrt{\frac{m\omega}{\hbar}} \qquad \psi_n(x) = \frac{\beta^{1/2}}{\pi^{1/4}} \frac{1}{\sqrt{2^n n!}} H_n(\beta x) e^{-\beta^2 x^2/2} \qquad E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

$$H_0(\beta x) = H_0(\xi) = 1 \qquad H_1(\beta x) = H_1(\xi) = 2\xi$$

$$H_2(\beta x) = H_2(\xi) = 4\xi^2 - 2 \qquad H_3(\beta x) = H_3(\xi) = 8\xi^3 - 12\xi$$

8 Position, Momentum, and Wavenumber Representations

$$p = \hbar k \qquad E_{\text{kinetic}} = E_T = \frac{\hbar^2 k^2}{2m}$$

$$|\Psi(p,t)|^2\, dp = |\Psi(k,t)|^2\, dk \qquad \Psi(p,t) = \frac{\Psi(k,t)}{\sqrt{\hbar}}$$

$$x_{\text{op}} = x \qquad p_{\text{op}} = \frac{\hbar}{i}\frac{\partial}{\partial x} \qquad Q\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}, t\right) \qquad \text{position representation}$$

$$x_{\text{op}} = -\frac{\hbar}{i}\frac{\partial}{\partial p} \qquad p_{\text{op}} = p \qquad Q\left(-\frac{\hbar}{i}\frac{\partial}{\partial p}, p, t\right) \qquad \text{momentum representation}$$

$$\delta(x) = \int_{-\infty}^{\infty} \frac{e^{ipx/\hbar}}{2\pi\hbar}\, dp \qquad \delta(x) = \int_{-\infty}^{\infty} \frac{e^{ikx}}{2\pi}\, dk$$

$$\Psi(x,t) = \int_{-\infty}^{\infty} \Psi(p,t) \frac{e^{ipx/\hbar}}{(2\pi\hbar)^{1/2}}\, dp \qquad \Psi(x,t) = \int_{-\infty}^{\infty} \Psi(k,t) \frac{e^{ikx}}{(2\pi)^{1/2}}\, dk$$

$$\Psi(p,t) = \int_{-\infty}^{\infty} \Psi(x,t) \frac{e^{-ipx/\hbar}}{(2\pi\hbar)^{1/2}}\, dx \qquad \Psi(k,t) = \int_{-\infty}^{\infty} \Psi(x,t) \frac{e^{-ikx}}{(2\pi)^{1/2}}\, dx$$

$$\Psi(\vec{r},t) = \int_{\text{all space}} \Psi(\vec{p},t) \frac{e^{i\vec{p}\cdot\vec{r}/\hbar}}{(2\pi\hbar)^{3/2}}\, d^3p \qquad \Psi(\vec{r},t) = \int_{\text{all space}} \Psi(\vec{k},t) \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}}\, d^3k$$

$$\Psi(\vec{p},t) = \int_{\text{all space}} \Psi(\vec{r},t) \frac{e^{-i\vec{p}\cdot\vec{r}/\hbar}}{(2\pi\hbar)^{3/2}}\, d^3r \qquad \Psi(\vec{k},t) = \int_{\text{all space}} \Psi(\vec{r},t) \frac{e^{-i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}}\, d^3r$$

9 Commutator Formulae

$$[A, BC] = [A,B]C + B[A,C] \qquad \left[\sum_i a_i A_i, \sum_j b_j B_j\right] = \sum_{i,j} a_i b_j [A_i, b_j]$$

$$\text{if} \qquad [B,[A,B]] = 0 \qquad \text{then} \qquad [A, F(B)] = [A,B]F'(B)$$

$$[x,p] = i\hbar \qquad [x, f(p)] = i\hbar f'(p) \qquad [p, g(x)] = -i\hbar g'(x)$$

$$[a, a^\dagger] = 1 \qquad [N, a] = -a \qquad [N, a^\dagger] = a^\dagger$$

---

10 Uncertainty Relations and Inequalities

$$\sigma_x \sigma_p = \Delta x \Delta p \geq \frac{\hbar}{2} \qquad \sigma_Q \sigma_Q = \Delta Q \Delta R \geq \frac{1}{2} \left| \langle i[Q, R] \rangle \right|$$

$$\sigma_H \Delta t_{\text{scale time}} = \Delta E \Delta t_{\text{scale time}} \geq \frac{\hbar}{2}$$

---

11 Probability Amplitudes and Probabilities

$$\Psi(x,t) = \langle x | \Psi(t) \rangle \qquad P(dx) = |\Psi(x,t)|^2 \, dx \qquad c_i(t) = \langle \phi_i | \Psi(t) \rangle \qquad P(i) = |c_i(t)|^2$$

---

12 Spherical Harmonics

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}} \qquad Y_{1,0} = \left(\frac{3}{4\pi}\right)^{1/2} \cos(\theta) \qquad Y_{1,\pm 1} = \mp \left(\frac{3}{8\pi}\right)^{1/2} \sin(\theta) e^{\pm i\phi}$$

$$L^2 Y_{\ell m} = \ell(\ell+1)\hbar^2 Y_{\ell m} \qquad L_z Y_{\ell m} = m\hbar Y_{\ell m} \qquad |m| \leq \ell \qquad m = -\ell, -\ell+1, \ldots, \ell-1, \ell$$

0	1	2	3	4	5	6	...
s	p	d	f	g	h	i	...

---

13 Hydrogenic Atom

$$\psi_{n\ell m} = R_{n\ell}(r) Y_{\ell m}(\theta, \phi) \qquad \ell \leq n-1 \qquad \ell = 0, 1, 2, \ldots, n-1$$

$$a_z = \frac{a}{Z}\left(\frac{m_e}{m_{\text{reduced}}}\right) \qquad a_0 = \frac{\hbar}{m_e c \alpha} = \frac{\lambda_{\text{C}}}{2\pi\alpha} \qquad \alpha = \frac{e^2}{\hbar c}$$

$$R_{10} = 2a_Z^{-3/2} e^{-r/a_Z} \qquad R_{20} = \frac{1}{\sqrt{2}} a_Z^{-3/2} \left(1 - \frac{1}{2}\frac{r}{a_Z}\right) e^{-r/(2a_Z)}$$

$$R_{21} = \frac{1}{\sqrt{24}} a_Z^{-3/2} \frac{r}{a_Z} e^{-r/(2a_Z)}$$

$$R_{n\ell} = -\left\{ \left(\frac{2}{na_Z}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3} \right\}^{1/2} e^{-\rho/2} \rho^\ell L_{n+\ell}^{2\ell+1}(\rho) \qquad \rho = \frac{2r}{nr_Z}$$

$$L_q(x) = e^x \left(\frac{d}{dx}\right)^q \left(e^{-x} x^q\right) \quad \text{Rodrigues's formula for the Laguerre polynomials}$$

$$L_q^j(x) = \left(\frac{d}{dx}\right)^j L_q(x) \qquad \text{Associated Laguerre polynomials}$$

$$\langle r\rangle_{n\ell m} = \frac{a_Z}{2}\left[3n^2 - \ell(\ell+1)\right]$$

$$\text{Nodes} = (n-1) - \ell \qquad \text{not counting zero or infinity}$$

$$E_n = -\frac{1}{2}m_e c^2\alpha^2\frac{Z^2}{n^2}\frac{m_{\text{reduced}}}{m_e} = -E_{\text{Ryd}}\frac{Z^2}{n^2}\frac{m_{\text{reduced}}}{m_e} = -13.606\frac{Z^2}{n^2}\frac{m_{\text{reduced}}}{m_e}\ \text{eV}$$

---

14 General Angular Momentum Formulae

$$[J_i, J_j] = i\hbar\varepsilon_{ijk}J_k \qquad \text{(Einstein summation on } k\text{)} \qquad [J^2, \vec{J}\,] = 0$$

$$J^2|jm\rangle = j(j+1)\hbar^2|jm\rangle \qquad J_z|jm\rangle = m\hbar|jm\rangle$$

$$J_\pm = J_x \pm iJ_y \qquad J_\pm|jm\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}|jm\pm 1\rangle$$

$$J_{\left\{ {x \atop y} \right\}} = \left\{ \begin{matrix} \frac{1}{2} \\ \frac{1}{2i} \end{matrix} \right\}(J_+ \pm J_-) \qquad J_\pm^\dagger J_\pm = J_\mp J_\pm = J^2 - J_z(J_z \pm \hbar)$$

$$[J_{fi}, J_{gj}] = \delta_{fg}i\hbar\varepsilon_{ijk}J_k \qquad \vec{J} = \vec{J}_1 + \vec{J}_2 \qquad J^2 = J_1^2 + J_2^2 + J_{1+}J_{2-} + J_{1-}J_{2+} + 2J_{1z}J_{2z}$$

$$J_\pm = J_{1\pm} + J_{2\pm} \qquad |j_1j_2jm\rangle = \sum_{m_1m_2,\, m=m_1+m_2} |j_1j_2m_1m_2\rangle\langle j_1j_2m_1m_2|j_1j_2jm\rangle j_1j_2jm\rangle$$

$$|j_1 - j_2| \le j \le j_1 + j_2 \qquad \sum_{|j_1-j_2|}^{j_1+j_2}(2j+1) = (2j_1+1)(2j_2+1)$$

---

15 Spin 1/2 Formulae

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$|\pm\rangle_x = \frac{1}{\sqrt{2}}\left(|+\rangle \pm |-\rangle\right) \qquad |\pm\rangle_y = \frac{1}{\sqrt{2}}\left(|+\rangle \pm i|-\rangle\right) \qquad |\pm\rangle_z = |\pm\rangle$$

$$|++\rangle = |1,+\rangle|2,+\rangle \qquad |+-\rangle = \frac{1}{\sqrt{2}}\left(|1,+\rangle|2,-\rangle \pm |1,-\rangle|2,+\rangle\right) \qquad |--\rangle = |1,-\rangle|2,-\rangle$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_i\sigma_j = \delta_{ij} + i\varepsilon_{ijk}\sigma_k \qquad [\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k \qquad \{\sigma_i, \sigma_j\} = 2\delta_{ij}$$

$$(\vec{A}\cdot\vec{\sigma})(\vec{B}\cdot\vec{\sigma}) = \vec{A}\cdot\vec{B} + i(\vec{A}\times\vec{B})\cdot\vec{\sigma}$$

$$\frac{d(\vec{S}\cdot\hat{n})}{d\alpha} = -\frac{i}{\hbar}[\vec{S}\cdot\hat{\alpha}, \vec{S}\cdot\hat{n}] \qquad \vec{S}\cdot\hat{n} = e^{-i\vec{S}\cdot\vec{\alpha}}\vec{S}\cdot\hat{n}_0 e^{i\vec{S}\cdot\vec{\alpha}} \qquad |\hat{n}_\pm\rangle = e^{-i\vec{S}\cdot\vec{\alpha}}|\hat{z}_\pm\rangle$$

$$e^{ixA} = \mathbf{1}\cos(x) + iA\sin(x) \quad \text{if } A^2 = \mathbf{1} \qquad\qquad e^{-i\vec{\sigma}\cdot\vec{\alpha}/2} = \mathbf{1}\cos(x) - i\vec{\sigma}\cdot\hat{\alpha}\sin(x)$$

$$\sigma_i f(\sigma_j) = f(\sigma_j)\sigma_i\delta_{ij} + f(-\sigma_j)\sigma_i(1-\delta_{ij})$$

$$\mu_{\text{Bohr}} = \frac{e\hbar}{2m} = 0.927400915(23)\times 10^{-24}\,\text{J/T} = 5.7883817555(79)\times 10^{-5}\,\text{eV/T}$$

$$g = 2\left(1 + \frac{\alpha}{2\pi} + \ldots\right) = 2.0023193043622(15)$$

$$\vec{\mu}_{\text{orbital}} = -\mu_{\text{Bohr}}\frac{\vec{L}}{\hbar} \qquad \vec{\mu}_{\text{spin}} = -g\mu_{\text{Bohr}}\frac{\vec{S}}{\hbar} \qquad \vec{\mu}_{\text{total}} = \vec{\mu}_{\text{orbital}} + \vec{\mu}_{\text{spin}} = -\mu_{\text{Bohr}}\frac{(\vec{L}+g\vec{S})}{\hbar}$$

$$H_\mu = -\vec{\mu}\cdot\vec{B} \qquad H_\mu = \mu_{\text{Bohr}}B_z\frac{(L_z + gS_z)}{\hbar}$$

16 Time-Independent Approximation Methods

$$H = H^{(0)} + \lambda H^{(1)} \qquad |\psi\rangle = N(\lambda)\sum_{k=0}^{\infty}\lambda^k|\psi_n^{(k)}\rangle$$

$$H^{(1)}|\psi_n^{(m-1)}\rangle(1-\delta_{m,0}) + H^{(0)}|\psi_n^{(m)}\rangle = \sum_{\ell=0}^{m}E^{(m-\ell)}|\psi_n^{(\ell)}\rangle \qquad |\psi_n^{(\ell>0)}\rangle = \sum_{m=0,\ m\neq n}^{\infty}a_{nm}|\psi_n^{(0)}\rangle$$

$$\begin{aligned}
|\psi_n^{\text{1st}}\rangle &= |\psi_n^{(0)}\rangle + \lambda\sum_{\text{all }k,\ k\neq n}\frac{\left\langle\psi_k^{(0)}|H^{(1)}|\psi_n^{(0)}\right\rangle}{E_n^{(0)} - E_k^{(0)}}|\psi_k^{(0)}\rangle \\
E_n^{\text{1st}} &= E_n^{(0)} + \lambda\left\langle\psi_n^{(0)}|H^{(1)}|\psi_n^{(0)}\right\rangle \\
E_n^{\text{2nd}} &= E_n^{(0)} + \lambda\left\langle\psi_n^{(0)}|H^{(1)}|\psi_n^{(0)}\right\rangle + \lambda^2\sum_{\text{all }k,\ k\neq n}\frac{\left|\left\langle\psi_k^{(0)}|H^{(1)}|\psi_n^{(0)}\right\rangle\right|^2}{E_n^{(0)} - E_k^{(0)}}
\end{aligned}$$

$$E(\phi) = \frac{\langle\phi|H|\phi\rangle}{\langle\phi|\phi\rangle} \qquad \delta E(\phi) = 0$$

$$H_{kj} = \langle \phi_k | H | \phi_j \rangle \qquad H\vec{c} = E\vec{c}$$

---

17 Time-Dependent Perturbation Theory

$$\pi = \int_{-\infty}^{\infty} \frac{\sin^2(x)}{x^2}\, dx$$

$$\Gamma_{0\to n} = \frac{2\pi}{\hbar} |\langle n | H_{\text{perturbation}} | 0 \rangle|^2 \delta(E_n - E_0)$$

---

18 Interaction of Radiation and Matter

$$\vec{E}_{\text{op}} = -\frac{1}{c}\frac{\partial \vec{A}_{\text{op}}}{\partial t} \qquad \vec{B}_{\text{op}} = \nabla \times \vec{A}_{\text{op}}$$

---

19 Box Quantization

$$kL = 2\pi n, \quad n = 0, \pm 1, \pm 2, \ldots \qquad k = \frac{2\pi n}{L} \qquad \Delta k_{\text{cell}} = \frac{2\pi}{L} \qquad \Delta k_{\text{cell}}^3 = \frac{(2\pi)^3}{V}$$

$$dN_{\text{states}} = g\frac{k^2\, dk\, d\Omega}{(2\pi)^3/V}$$

---

20 Identical Particles

$$|a, b\rangle = \frac{1}{\sqrt{2}}\left(|1, a; 2, b\rangle \pm |1, b; 2, a\rangle\right)$$

$$\psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}\left(\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) \pm \psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\right)$$

---

21 Second Quantization

$$[a_i, a_j^\dagger] = \delta_{ij} \qquad [a_i, a_j] = 0 \qquad [a_i^\dagger, a_j^\dagger] = 0 \qquad |N_1, \ldots, N_n\rangle = \frac{(a_n^\dagger)^{N_n}}{\sqrt{N_n!}} \cdots \frac{(a_1^\dagger)^{N_1}}{\sqrt{N_1!}} |0\rangle$$

$$\{a_i, a_j^\dagger\} = \delta_{ij} \qquad \{a_i, a_j\} = 0 \qquad \{a_i^\dagger, a_j^\dagger\} = 0 \qquad |N_1, \ldots, N_n\rangle = (a_n^\dagger)^{N_n} \ldots (a_1^\dagger)^{N_1} |0\rangle$$

$$\Psi_s(\vec{r})^\dagger = \sum_{\vec{p}} \frac{e^{-i\vec{p}\cdot\vec{r}}}{\sqrt{V}} a_{\vec{p}s}^\dagger \qquad \Psi_s(\vec{r}) = \sum_{\vec{p}} \frac{e^{i\vec{p}\cdot\vec{r}}}{\sqrt{V}} a_{\vec{p}s}$$

$$[\Psi_s(\vec{r}), \Psi_{s'}(\vec{r}\,')]_\mp = 0 \qquad [\Psi_s(\vec{r})^\dagger, \Psi_{s'}(\vec{r}\,')^\dagger]_\mp = 0 \qquad [\Psi_s(\vec{r}), \Psi_{s'}(\vec{r}\,')^\dagger]_\mp = \delta(\vec{r} - \vec{r}\,')\delta_{ss'}$$

$$|\vec r_1 s_1,\ldots,\vec r_n s_n\rangle = \frac{1}{\sqrt{n!}}\Psi_{s_n}(\vec r_n)^\dagger \ldots \Psi_{s_n}(\vec r_n)^\dagger|0\rangle$$

$$\Psi_s(\vec r)^\dagger|\vec r_1 s_1,\ldots,\vec r_n s_n\rangle\sqrt{n+1}|\vec r_1 s_1,\ldots,\vec r_n s_n,\vec r s\rangle$$

$$|\Phi\rangle = \int d\vec r_1\ldots d\vec r_n\,\Phi(\vec r_1,\ldots,\vec r_n)|\vec r_1 s_1,\ldots,\vec r_n s_n\rangle$$

$$1_n = \sum_{s_1\ldots s_n}\int d\vec r_1\ldots d\vec r_n\,|\vec r_1 s_1,\ldots,\vec r_n s_n\rangle\langle\vec r_1 s_1,\ldots,\vec r_n s_n| \qquad 1 = |0\rangle\langle 0| + \sum_{n=1}^{\infty} 1_n$$

$$N = \sum_{\vec p s} a^\dagger_{\vec p s} a_{\vec p s} \qquad T = \sum_{\vec p s}\frac{p^2}{2m} a^\dagger_{\vec p s} a_{\vec p s}$$

$$\rho_s(\vec r) = \Psi_s(\vec r)^\dagger\Psi_s(\vec r) \qquad N = \sum_s\int d\vec r\,\rho_s(\vec r) \qquad T = \frac{1}{2m}\sum_s\int d\vec r\,\nabla\Psi_s(\vec r)^\dagger\cdot\nabla\Psi_s(\vec r)$$

$$\vec j_s(\vec r) = \frac{1}{2im}\left[\Psi_s(\vec r)^\dagger\nabla\Psi_s(\vec r) - \Psi_s(\vec r)\nabla\Psi_s(\vec r)^\dagger\right]$$

$$G_s(\vec r - \vec r\,') = \frac{3n}{2}\frac{\sin(x) - x\cos(x)}{x^3} \qquad g_{ss'}(\vec r - \vec r\,') = 1 - \delta_{ss'}\frac{G_s(\vec r - \vec r\,')^2}{(n/2)^2}$$

$$v_{\text{2nd}} = \frac{1}{2}\sum_{ss'}\int d\vec r d\vec r\,'\,v(\vec r - \vec r\,')\Psi_s(\vec r)^\dagger\Psi_{s'}(\vec r\,')^\dagger\Psi_{s'}(\vec r\,')\Psi_s(\vec r)$$

$$v_{\text{2nd}} = \frac{1}{2V}\sum_{pp'qq'}\sum_{ss'} v_{\vec p-\vec p\,'}\delta_{\vec p+\vec q,\vec p\,'+\vec q\,'} a^\dagger_{\vec p s} a^\dagger_{\vec q s'} a_{\vec q\,' s'} a_{\vec p\,' s} \qquad v_{\vec p-\vec p\,'} = \int d\vec r\, e^{-i(\vec p-\vec p\,')\cdot\vec r} v(\vec r)$$

---

22 **Klein-Gordon Equation**

$$E = \sqrt{p^2c^2 + m^2c^4} \qquad \frac{1}{c^2}\left(i\hbar\frac{\partial}{\partial t}\right)^2\Psi(\vec r,t) = \left[\left(\frac{\hbar}{i}\nabla\right)^2 + m^2c^2\right]\Psi(\vec r,t)$$

$$\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 + \left(\frac{mc}{\hbar}\right)^2\right]\Psi(\vec r,t) = 0$$

$$\rho = \frac{i\hbar}{2mc^2}\left(\Psi^*\frac{\partial\Psi}{\partial t} - \Psi\frac{\partial\Psi^*}{\partial t}\right) \qquad \vec j = \frac{\hbar}{2im}\left(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\right)$$

$$\frac{1}{c^2}\left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)^2\Psi(\vec r,t) = \left[\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec A\right)^2 + m^2c^2\right]\Psi(\vec r,t)$$

$$\Psi_+(\vec p,E) = e^{i(\vec p\cdot\vec r - Et)/\hbar} \qquad \Psi_-(\vec p,E) = e^{-i(\vec p\cdot\vec r - Et)/\hbar}$$

Appendix 3 Multiple-Choice Problem Answer Tables

Note: For those who find scantrons frequently inaccurate and prefer to have their own table and marking template, the following are provided. I got the template trick from Neil Huffacker at University of Oklahoma. One just punches out the right answer places on an answer table and overlays it on student answer tables and quickly identifies and marks the wrong answers

Answer Table for the Multiple-Choice Questions

	a	b	c	d	e		a	b	c	d	e
1.	O	O	O	O	O	6.	O	O	O	O	O
2.	O	O	O	O	O	7.	O	O	O	O	O
3.	O	O	O	O	O	8.	O	O	O	O	O
4.	O	O	O	O	O	9.	O	O	O	O	O
5.	O	O	O	O	O	10.	O	O	O	O	O

Answer Table for the Multiple-Choice Questions

	a	b	c	d	e		a	b	c	d	e
1.	O	O	O	O	O	11.	O	O	O	O	O
2.	O	O	O	O	O	12.	O	O	O	O	O
3.	O	O	O	O	O	13.	O	O	O	O	O
4.	O	O	O	O	O	14.	O	O	O	O	O
5.	O	O	O	O	O	15.	O	O	O	O	O
6.	O	O	O	O	O	16.	O	O	O	O	O
7.	O	O	O	O	O	17.	O	O	O	O	O
8.	O	O	O	O	O	18.	O	O	O	O	O
9.	O	O	O	O	O	19.	O	O	O	O	O
10.	O	O	O	O	O	20.	O	O	O	O	O

Answer Table for the Multiple-Choice Questions

	a	b	c	d	e		a	b	c	d	e
1.	O	O	O	O	O	16.	O	O	O	O	O
2.	O	O	O	O	O	17.	O	O	O	O	O
3.	O	O	O	O	O	18.	O	O	O	O	O
4.	O	O	O	O	O	19.	O	O	O	O	O
5.	O	O	O	O	O	20.	O	O	O	O	O
6.	O	O	O	O	O	21.	O	O	O	O	O
7.	O	O	O	O	O	22.	O	O	O	O	O
8.	O	O	O	O	O	23.	O	O	O	O	O
9.	O	O	O	O	O	24.	O	O	O	O	O
10.	O	O	O	O	O	25.	O	O	O	O	O
11.	O	O	O	O	O	26.	O	O	O	O	O
12.	O	O	O	O	O	27.	O	O	O	O	O
13.	O	O	O	O	O	28.	O	O	O	O	O
14.	O	O	O	O	O	29.	O	O	O	O	O
15.	O	O	O	O	O	30.	O	O	O	O	O

NAME:

Answer Table for the Multiple-Choice Questions

	a	b	c	d	e		a	b	c	d	e
1.	O	O	O	O	O	21.	O	O	O	O	O
2.	O	O	O	O	O	22.	O	O	O	O	O
3.	O	O	O	O	O	23.	O	O	O	O	O
4.	O	O	O	O	O	24.	O	O	O	O	O
5.	O	O	O	O	O	25.	O	O	O	O	O
6.	O	O	O	O	O	26.	O	O	O	O	O
7.	O	O	O	O	O	27.	O	O	O	O	O
8.	O	O	O	O	O	28.	O	O	O	O	O
9.	O	O	O	O	O	29.	O	O	O	O	O
10.	O	O	O	O	O	30.	O	O	O	O	O
11.	O	O	O	O	O	31.	O	O	O	O	O
12.	O	O	O	O	O	32.	O	O	O	O	O
13.	O	O	O	O	O	33.	O	O	O	O	O
14.	O	O	O	O	O	34.	O	O	O	O	O
15.	O	O	O	O	O	35.	O	O	O	O	O
16.	O	O	O	O	O	36.	O	O	O	O	O
17.	O	O	O	O	O	37.	O	O	O	O	O
18.	O	O	O	O	O	38.	O	O	O	O	O
19.	O	O	O	O	O	39.	O	O	O	O	O
20.	O	O	O	O	O	40.	O	O	O	O	O

Answer Table

Name:

	a	b	c	d	e
1.	O	O	O	O	O
2.	O	O	O	O	O
3.	O	O	O	O	O
4.	O	O	O	O	O
5.	O	O	O	O	O
6.	O	O	O	O	O
7.	O	O	O	O	O
8.	O	O	O	O	O
9.	O	O	O	O	O
10.	O	O	O	O	O
11.	O	O	O	O	O
12.	O	O	O	O	O
13.	O	O	O	O	O
14.	O	O	O	O	O
15.	O	O	O	O	O
16.	O	O	O	O	O
17.	O	O	O	O	O
18.	O	O	O	O	O
19.	O	O	O	O	O
20.	O	O	O	O	O
21.	O	O	O	O	O
22.	O	O	O	O	O
23.	O	O	O	O	O
24.	O	O	O	O	O
25.	O	O	O	O	O
26.	O	O	O	O	O
27.	O	O	O	O	O
28.	O	O	O	O	O
29.	O	O	O	O	O
30.	O	O	O	O	O

	a	b	c	d	e
31.	O	O	O	O	O
32.	O	O	O	O	O
33.	O	O	O	O	O
34.	O	O	O	O	O
35.	O	O	O	O	O
36.	O	O	O	O	O
37.	O	O	O	O	O
38.	O	O	O	O	O
39.	O	O	O	O	O
40.	O	O	O	O	O
41.	O	O	O	O	O
42.	O	O	O	O	O
43.	O	O	O	O	O
44.	O	O	O	O	O
45.	O	O	O	O	O
46.	O	O	O	O	O
47.	O	O	O	O	O
48.	O	O	O	O	O
49.	O	O	O	O	O
50.	O	O	O	O	O
51.	O	O	O	O	O
52.	O	O	O	O	O
53.	O	O	O	O	O
54.	O	O	O	O	O
55.	O	O	O	O	O
56.	O	O	O	O	O
57.	O	O	O	O	O
58.	O	O	O	O	O
59.	O	O	O	O	O
60.	O	O	O	O	O