Quantum Mechanics II

Final Exam   2011 May 11, Wednesday

NAME: SIGNATURE:

Instructions: There are 40 multiple-choice questions each worth 1 mark for a total of 40 marks altogether. Choose the **BEST** answer, completion, etc., and darken fully the appropriate circle on the table provided on the next page. Read all responses carefully. **NOTE** long detailed preambles and responses won't depend on hidden keywords: keywords in such preambles and responses are bold-faced capitalized.

There are **FOUR** full answer questions each worth 10 marks for a total of 40 marks altogether. Answer them all on the paper provided. It is important that you **SHOW** (**SHOW, SHOW, SHOW**) how you got the answer.

This is a **CLOSED-BOOK** exam. **NO** cheat sheets allowed. An equation sheet is provided. Calculators are permitted for calculations. Cell phones **MUST** be turned off. The test is out of 80 marks altogether.

This a 2-hour test. Remember your name (and write it down on the exam too).

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

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.

   SUGGESTED ANSWER: (c)

   Wikipedia confirms this definition of a central force. Mathemetically, one can write the force

   $$\vec{F}(\vec{r}) = F(r)\hat{r} \ .$$

   But what would a force like

   $$\vec{F}(\vec{r}) = F(\vec{r})\hat{r}$$

   be called. It's not officially a central force since the magnitude depends on direction. But its torque about the center is also zero, and so it conserves angular momentum. Perhaps, such forces are rare, and therefore not much studied.

   Wrong Answers:
   a) Nah.
   b) Exactly wrong.

   Redaction: Jeffery, 2001jan01

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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.

   SUGGESTED ANSWER: (b) Yes separation of variables is the conventional name. See Ar-86.

   Wrong Answers:
   e) A nonsense answer

   Redaction: Jeffery, 2001jan01

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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

   $$\mathrm{LHS}(x) = \mathrm{RHS}(y) \ ,$$

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.

SUGGESTED ANSWER: (c)

In quantum mechanics, it is a postulate that a complete set of eigenstates exists for any observable and that any physical state defined for the same space as the observable can be expanded exactly in those eigenstates in principle. The whole paradigm of quantum mechanics relies on this postulate—and quantum mechanics has never failed.

Wrong answers:
  d) Seems reasonable.
  e) Metaphorical names due turn up in physics like the Monte Carlo method (named after a famous casino in Monaco) and the Urca process (named after a casino in Rio de Janeiro). One sometimes gets the feeling that theoretical physicists spend a lot of time in casinos. I used to wander through them all the time in my Vegas years.

Redaction: Jeffery, 2008jan01

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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.

SUGGESTED ANSWER: (c)

In quantum mechanics, it is a postulate that a complete set of eigenstates exists for any observable and that any physical state defined for the same space as the observable can be expanded exactly in those eigenstates in principle. The whole paradigm of quantum mechanics relies on this postulate—and quantum mechanics has never failed. Thus, separation of the variables when it can be applied to quantum mechanics is a very important procedure.

Wrong answers:
  d) Seems reasonable.
  e) Metaphorical names due turn up in physics like the Monte Carlo method (named after a famous casino in Monaco) and the Urca process (named after a casino in Rio de Janeiro). One sometimes gets the feeling that theoretical physicists spend a lot of time in casinos. I used to wander through them all the time in my Vegas years.

Redaction: Jeffery, 2008jan01

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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

SUGGESTED ANSWER: (b)

Wrong answers:
   e) Seems a bit pointless.

Redaction: Jeffery, 2001jan01

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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) $m = \dfrac{1}{m_1}$.

SUGGESTED ANSWER: (d) See Gr-202 and 2011 notes 5-77.

   The formula originates in reducing a two-body problem to a one-body problem. One gets

$$\frac{1}{m} = \frac{1}{m_1} + \frac{1}{m_2}$$

from which

$$m = \begin{cases} \dfrac{m_1 m_2}{m_1 + m_2} & \text{in general;} \\[2ex] \dfrac{m_2}{1 + m_2/m_1} \approx m_2 \left(1 - \dfrac{m_2}{m_1}\right) & \text{for } m_2 << m_1; \\[2ex] \dfrac{m_1}{2} & \text{for } m_1 = m_2. \end{cases}$$

Wrong Answers:
   a) Dimensionally wrong.
   b) Dimensionally wrong.
   c) Dimensionally wrong.
   e) Dimensionally wrong and it only refers to one mass.

Redaction: Jeffery, 2001jan01

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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.

SUGGESTED ANSWER: (b)

Wrong Answers:
   d) Legend has it that Pythagoras discovered the harmonic properties of strings.
   e) Vincenzo Galileo, father of the other Galileo, was a scientist too and studied music scientifically.

Redaction: Jeffery, 2001jan01

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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

   SUGGESTED ANSWER: (d)

   Wrong answers:
   a) These turn up as factors in the solution of the 1-dimensional simple harmonic oscillator problem.
   c) These turn up as factors in the solution of the radial part part of the Coulomb potential 2-body problem
   e) These have uses in numerical computation.

   Redaction: Jeffery, 2008jan01

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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) $2a^{-3/2}e^{-r/a}$.

   SUGGESTED ANSWER: (c)

   Wrong Answers:
   a) This is the general azimuthal component of the spherical harmonics: $m = 0, \pm 1, \pm 2, \ldots, \pm \ell$.
   b) This is radial and it's not normalizable.
   d) Except for Y_{00} itself, the spherical harmonics are all combinations of sinusoidal functions of the θ and ϕ.
   e) This is the R_{10} hydrogenic radial wave function where a is the scale radius
   $$a = a_0 \frac{m_e}{m} \frac{1}{Z} \ ,$$
   where m_e is the electron mass, m is the reduced mass, Z is the number of unit charges of the central particle, and a_0 is the Bohr radius (Gr2005-137). The Bohr radius in MKS units is given by
   $$a_0 = \frac{\hbar^2}{m_e[e^2/(4\pi\varepsilon_0)]} = \frac{\lambda_C}{2\pi} \frac{1}{\alpha} = 0.52917720859(36) \, \text{Å} \ ,$$
   where e is the elementary charge, $\lambda_C = \hbar/(m_e c)$ is the Compton wavelength, and $\alpha \approx /137$ is the fine structure constant.

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011 qmult 00500 1 4 2 easy deducto-memory: spdf designations

10. Conventionally, the spherical harmonic eigenstates for angular momentum quantum numbers

$$\ell = 0, 1, 2, 3, 4, ...$$

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) $@%&*!!

SUGGESTED ANSWER: (b)

Wrong Answers:
   a) This is the way it should be, not the way it is.
   e) Only in Tasmanian devilish.

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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

SUGGESTED ANSWER: (c)

Wrong answers:
   b) A British rock band of the 1960s: not the Beatles.
   d) These are the $\ell = 1$ electrons.
   e) These are the $\ell = 5$ electrons.

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019 qmult 00100 1 4 5 easy deducto-memory: symmetrization principle

12. "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

$$\psi_{\mathrm{new}}(\vec{r}_1 m_1, \vec{r}_2 m_2) = \psi(\vec{r}_2 m_2, \vec{r}_1 m_1) \ .$$

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

$$\psi_{\mathrm{com}}(\vec{r}_1 m_1, \vec{r}_2 m_2) = c_i \psi(\vec{r}_1 m_1, \vec{r}_2 m_2) + c_j \psi(\vec{r}_2 m_2, \vec{r}_1 m_1)$$

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 $\psi_{\mathrm{com}}(\vec{r}_1 m_1, \vec{r}_2 m_2)$ be normalized. In quantum mechanics, $\psi_{\mathrm{com}}(\vec{r}_1 m_1, \vec{r}_2 m_2)$ 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

$$
\begin{aligned}
\psi_{\text{com}}(\vec{r}_1 m_1, \vec{r}_2 m_2) &= c_i \psi(\vec{r}_1 m_1, \vec{r}_2 m_2) + c_j \psi(\vec{r}_2 m_2, \vec{r}_1 m_1) \\
&= c_i \psi(\vec{r}_1 m_1, \vec{r}_2 m_2) + c_j e^{i\phi}\psi(\vec{r}_1 m_1, \vec{r}_2 m_2) \\
&= (c_i + c_j e^{i\phi})\psi(\vec{r}_1 m_1, \vec{r}_2 m_2)
\end{aligned}
$$

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 $e^{i\phi} = \pm 1$ 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 $e^{i\phi} = \pm 1$ 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

SUGGESTED ANSWER: (e)

Longwinded, but the symmetrization principle really can't be fully described by a single sentence.

Wrong answers:
    d) Wigner's last stand?

Redaction: Jeffery, 2001jan01

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019 qmult 00110 1 1 3 easy memory: exchange degeneracy and symmetrization principle
13. 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.

SUGGESTED ANSWER: (c)

Wrong answers:
    e) By Gad, Holmes, baffled again.

Redaction: Jeffery, 2008jan01

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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

14. "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

SUGGESTED ANSWER: (e) See Wikipedia: Bose-Einstein condensate.

Wrong answers:
    c) Rabi-Schwinger-Baym-Sutherland-Jeffery is my Ph.D. pedigree: sort of like that of a dog. Obviously things have gone downhill in the last step anyhow. The descent of Ph.D.'s and proto-Ph.D.'s must go back to the Ur-Ph.D.—probably Thales.

Redaction: Jeffery, 2001jan01

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022 qmult 00100 1 1 3 easy memory: simplest quantum mechanical solid model
15. 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.

SUGGESTED ANSWER: (c)

The free electron gas model of a solid was developed by Arnold Sommerfeld (1868–1951) starting in 1927 shortly after the discovery of quantum mechanics in 1926 or so. The free electron gas model was developed starting from Drude classical free electron gas model. Sommerfeld was getting on in years when he developed the free electron gas models. It's proof that older physicists/dogs can sometimes learn new tricks.

Wrong answers:
  a) A nonsense answer.

Redaction: Jeffery, 2008jan01

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022 qmult 00110 1 1 1 easy memory: infinite square boundary conditions
16. 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

SUGGESTED ANSWER: (a)

Wrong answers:
  b) These can be used and must be used, I imagine, in some cases. But they are not a simple choice.

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022 qmult 00130 1 4 4 easy deducto-memory: periodic boundary conditions
Extra keywords: mathematical physics

17. "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

SUGGESTED ANSWER: (d)

Wrong answers:
 a) Exactly wrong.
 b) Exactly wrong.
 c) I.I. Rabi (1898–1988), Julian Schwinger (1918–1994), Gordon Baym (circa 1935–), Peter Sutherland (circa 1945–) to well me: my Ph.D. pedigree.

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023 qmult 00240 1 1 3 easy memory: statistical weight formulae
Extra keywords: See Gr-234–235

18. 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.

SUGGESTED ANSWER: (c)

Wrong answers:
 e) A nonsense answer.

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023 qmult 00330 1 4 1 easy deducto-memory: Lagrance multipliers
Extra keywords: mathematical physics

19. "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

SUGGESTED ANSWER: (a)

Wrong answers:
a) As Lurch would say AAAARGH.

Redaction: Jeffery, 2008jan01

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023 qmult 00340 1 1 3 easy memory: Lagrange multiplier formula for W
20. 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 $W \leq 0$

SUGGESTED ANSWER: (c)

Actually, we do have the constraint all $N_i \geq 0$, but that constraint is not built into the Lagrange multiplier procedure for finding the N_i values that maximize W.

Wrong answers:
a) A nonsense answer.

Redaction: Jeffery, 2008jan01

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023 qmult 00350 1 4 5 easy deducto-memory: Stirling's series
Extra keywords: mathematical physics

21. "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

SUGGESTED ANSWER: (e) See Arf-464. Actually Robert invented the engine and James the series—but they were both Scots.

Wrong answers:
  a) ICE is for internal combustion engine.

Redaction: Jeffery, 2008jan01

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023 qmult 00352 1 1 5 easy memory: ln of factorials difference
22. The difference

$$\ln(z!) - \ln[(z-1)!]$$

equals:

a) $\ln(z-1)$.   b) $\ln(z!)$.   c) $z - 1$.   d) z.   e) $\ln(z)$.

SUGGESTED ANSWER: (e)

Behold:

$$\ln(z!) - \ln[(z-1)!] = \ln(z) + \ln[(z-1)!] - \ln[(z-1)!] = \ln(z) \ .$$

Wrong answers:
  b) Does this seem likely?

Redaction: Jeffery, 2008jan01

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023 qmult 00410 1 1 2 easy memory: stat mech entropy
23. 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.

SUGGESTED ANSWER: (b)

Wrong answers:
  a) A nonsense answer.

Redaction: Jeffery, 2008jan01

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023 qmult 00490 1 1 4 easy memory: stat mech distribution formulae
    Extra keywords: GR-241
24. 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

SUGGESTED ANSWER: (d)

Wrong answers:
  e) A nonsense answer.

Redaction: Jeffery, 2008jan01

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023 qmult 00530 1 1 1 easy memory: MB average energy per particle
25. 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) $E_{\text{ave}} = \dfrac{3}{2}kT$ b) $E_{\text{ave}} = \dfrac{1}{2}kT$ c) $E_{\text{ave}} = kT$ d) $E_{\text{ave}} = \dfrac{3}{5}E_{\text{Fermi}}$
  e) $E_{\text{ave}} = E_{\text{Fermi}}$

SUGGESTED ANSWER: (a)

  Behold:

$$E_{\text{ave}} = \frac{\int_0^\infty E e^{-E/(kT)} E^{1/2} \, dE}{\int_0^\infty e^{-E/(kT)} E^{1/2} \, dE} = kT \frac{(3/2)!}{(1/2)!} = \frac{3}{2}kT \ ,$$

where we note that the chemical potential μ has canceled out.
    See Arf-453 and Gr-241.

Wrong answers:
  a) A nonsense answer.

Redaction: Jeffery, 2008jan01

023 qmult 00540 1 1 1 easy memory: Maxwell-Boltzmann chemical potential
 Extra keywords: Need the factorial function, and so give question 530 first.
 26. 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) $\mu = kT \ln \left\{ \dfrac{n}{g \left[mkT / \left(2\pi \hbar^2 \right) \right]^{3/2}} \right\}$

b) $\mu = kT \ln \left\{ \dfrac{n}{g \left[2mkT / \left(\pi \hbar^2 \right) \right]^{3/2}} \right\}$ c) $\mu = \ln \left\{ \dfrac{n}{g \left[mkT / \left(2\pi \hbar^2 \right) \right]^{3/2}} \right\}$

d) $\mu = kT \ln \left\{ \dfrac{n}{g \left[(3/2)mkT / \left(\pi \hbar^2 \right) \right]^{3/2}} \right\}$

e) $\mu = \ln \left\{ \dfrac{n}{g \left[2mkT / \left(\pi \hbar^2 \right) \right]^{3/2}} \right\}$

SUGGESTED ANSWER: (a)

 Behold:

$$n = \int_0^\infty e^{-(E-\mu)/(kT)} \frac{g}{(2\pi)^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} E^{1/2}\, dE$$

$$= e^{\mu/(kT)} \frac{g}{(2\pi)^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \int_0^\infty e^{-E/(kT)} E^{1/2}\, dE$$

$$= e^{\mu/(kT)} \frac{g}{(2\pi)^2} \left(\frac{2mkT}{\hbar^2} \right)^{3/2} \int_0^\infty e^{-z} x^{1/2}\, dx$$

$$= e^{\mu/(kT)} \frac{g}{(2\pi)^2} \left(\frac{2mkT}{\hbar^2} \right)^{3/2} \left(\frac{1}{2} \right)!$$

$$= e^{\mu/(kT)} \frac{g}{(2\pi)^2} \left(\frac{2mkT}{\hbar^2} \right)^{3/2} \frac{\sqrt{\pi}}{2}$$

$$= e^{\mu/(kT)} g \left(\frac{mkT}{2\pi \hbar^2} \right)^{3/2} \quad .$$

We invert this to obtain

$$\mu = kT \ln \left\{ \frac{n}{g \left[mkT / \left(2\pi\hbar^2 \right) \right]^{3/2}} \right\}$$

(Gr-242).

Wrong answers:
  c) Dimensionally incorrect.
  d) Dimensionally incorrect.

Redaction: Jeffery, 2008jan01

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023 qmult 00820 1 1 3 easy memory: Planck law
27. 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.

SUGGESTED ANSWER: (c) The formula is called the Planck law or the blackbody law (Wikipedia: Planck's law).

Wrong answers:
  a) Is this likely with that -1 in the denominator.

Redaction: Jeffery, 2008jan01

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023 qmult 00830 1 1 2 easy memory: hohlraum
28. 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.

SUGGESTED ANSWER: (b) The blackbody radiation is the emission from a nearly perfect Bose-Einstein gas, in fact.

Wrong answers:
  a) Is this likely for radiation field made up of photons?

Redaction: Jeffery, 2008jan01

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023 qmult 00840 1 1 3 easy memory: Wien's law

29. 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) $\dfrac{kTc}{\lambda^4}$.   b) $\dfrac{2kTc}{\lambda^4}$.   c) $\dfrac{2hc^2}{\lambda^5} e^{-hc/(\lambda kT)}$.   d) $\dfrac{kTc}{2\lambda^4}$.

e) $\dfrac{2hc^2}{\lambda^5} e^{hc/(\lambda kT)}$.

SUGGESTED ANSWER: (c)

If λ becomes sufficiently small (i.e., ν sufficiently large), then

$$e^{hc/(\lambda kT)} >> 1$$

and it is clear the answer (c) is correct (Wikipedia: Wein approximation).

Wrong answers:
 a) A nonsense answer.

Redaction: Jeffery, 2008jan01

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023 qmult 00842 1 1 2 easy memory: Rayleigh-Jeans law
30. 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) $\dfrac{2hc^2}{\lambda^5} e^{hc/(\lambda kT)}$.

SUGGESTED ANSWER: (b)

For long wavelengths,

$$\begin{aligned}
B_\lambda &= \frac{2hc^2}{\lambda^5} \frac{1}{e^{hc/(\lambda kT)} - 1} \approx \frac{2hc^2}{\lambda^5} \frac{1}{1 + hc/(\lambda kT) - 1} \\
&\approx \frac{2hc^2}{\lambda^5} \frac{1}{hc/(\lambda kT)} \\
&\approx \frac{2kTc}{\lambda^4}
\end{aligned}$$

(Wikipedia: Rayleigh-Jeans law).

Wrong answers:
 a) A nonsense answer.

Redaction: Jeffery, 2008jan01

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023 qmult 00850 1 1 1 easy memory: approximate solution Planck law stationary points

31. The function

$$f(x) = \frac{x^p}{e^x - 1}$$

for $x \geq 0$ and $p \gg 1$ has the approximate maximizing value:

   a) p.   b) $p/2$.   c) $1/p$.   d) p^2.   e) $\ln(p)$.

SUGGESTED ANSWER: (a)

   Behold:

$$\frac{df}{dx} = \frac{px^{p-1}}{e^x - 1} - \frac{x^p e^x}{(e^x - 1)^2}$$
$$= \frac{x^{p-1} e^x}{(e^x - 1)^2}[p(1 - e^{-x}) - x]$$

We find the interation equation for $df/dx = 0$ to be

$$x = p(1 - e^{-x}) \ .$$

If $p \gg 1$, then $e^{-p} \ll 1$ and the iteration equation is approximately solved by $x = p$. The derivative for $p \gg 1$ is clearly positive for x sufficiently small since

$$\frac{df}{dx}(x \ll 1) \approx \frac{x^{p-1} e^x}{(e^x - 1)^2}[x(p - 1)]$$

and negative for x sufficiently large since

$$\frac{df}{dx}(x \gg p) \approx \frac{x^{p-1} e^x}{(e^x - 1)^2}(p - x) \ .$$

Thus, the approximate stationary point must be a maximizing point.

Wrong answers:
   a) A nonsense answer.

Redaction: Jeffery, 2008jan01

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015 qmult 00090 1 1 1 easy memory: quantum perturbation Santa
   Extra keywords: the Christmas question

32. 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.

SUGGESTED ANSWER: (a) This is the Christmas question, but it will do for the spring commencement too.

Wrong Answers:

e) I'll take it.

Redaction: Jeffery, 2001jan01

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015 qmult 00100 1 1 1 easy memory: time-independent perturbation

33. 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.

SUGGESTED ANSWER: (a)

Wrong Answers:

b) A time-dependent system can have eigenstates and eigen-energies only at an instant in time I think. This is a useful concept I think, but it is not a best answer.

Redaction: Jeffery, 2001jan01

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015 qmult 00200 1 1 5 easy memory: zeroth order perturbation

34. 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.

SUGGESTED ANSWER: (e)

Wrong Answers:

b) Not grammatical, although Shakespeare got away with "most kindest" describing, I think, Julius Caesar.

Redaction: Jeffery, 2001jan01

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015 qmult 00300 1 1 2 easy memory: 1st order corrected energy

35. The formula

$$E_n^{\text{1st}} = E_n^{(0)} + \lambda \langle \psi_n^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle$$

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.

SUGGESTED ANSWER: (b)

Wrong Answers:
d) Just checking if you are awake.

Redaction: Jeffery, 2001jan01

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015 qmult 00400 1 4 4 easy deducto-memory: 1st order corrected state
36. The formula

$$|\psi_n^{\text{1st}}\rangle = |\psi_n^{(0)}\rangle + \lambda \sum_{\text{all } k, \text{ except } k \neq n} \frac{\langle \psi_k^{(0)}|H^{(1)}|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}}|\psi_k^{(0)}\rangle$$

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.

SUGGESTED ANSWER: (d)

Wrong Answers:
e) There's only 1 power of λ in the expression.

Redaction: Jeffery, 2001jan01

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015 qmult 00500 1 1 3 easy memory: 2nd order corrected energy
37. The formula

$$E_n^{\text{2nd}} = E_n^{(0)} + \lambda\langle \psi_n^{(0)}|H^{(1)}|\psi_n^{(0)}\rangle + \lambda^2 \sum_{\text{all } k, \text{ except } k \neq n} \frac{|\langle \psi_k^{(0)}|H^{(1)}|\psi_n^{(0)}\rangle|^2}{E_n^{(0)} - E_k^{(0)}}$$

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.

SUGGESTED ANSWER: (c)

Wrong Answers:
d) It's an energy quantity for crying out loud.

Redaction: Jeffery, 2001jan01

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015 qmult 00600 1 4 1 easy deducto-memory: degeneracy and perturbation
38. "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

SUGGESTED ANSWER: (a)

Wrong answers:
  d) Seemed likely to me too.

Redaction: Jeffery, 2001jan01

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015 qmult 01000 1 4 5 easy deducto-memory: diagonalization
  Extra keywords: mathematical physics
39. "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

SUGGESTED ANSWER: (e)

Wrong answers:
a) Exactly wrong.

Redaction: Jeffery, 2008jan01

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015 qmult 01020 1 1 2 easy memory: 2x2 eigenvalues
40. 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.

SUGGESTED ANSWER: (b)

Wrong answers:
c) There are only eigen-energies, and so the matrix is a 2×2 matrix.

Redaction: Jeffery, 2008jan01

011 qfull 00100 2 5 0 moderate thinking: 2-body reduced to 1-body problem
   Extra keywords: (Gr-178:5.1)

41. The 2-body time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m_1}\nabla_1^2\psi - \frac{\hbar^2}{2m_2}\nabla_2^2\psi + V_{\text{tot}}\psi = E_{\text{total}}\psi \ .$$

If the potential $V_{\text{tot}} = V(\vec{r}) + V_{\text{cm}}(\vec{R})$ (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 ∇_{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 ∇_{cm}^2 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 $V_{\text{tot}} = V(\vec{r}) + V_{\text{cm}}(\vec{R})$. Show explicitly how the separation of variables is done. What are the solutions of the center-of-mass problem if $V_{\text{cm}}(\vec{R}) = 0$? How would you interpret the solutions of the relative problem? **HINT:** I'm only looking for a short answer to the interpretation question.

SUGGESTED ANSWER:

a) Well substituting for $\vec{r}_2$ using expression $\vec{r}_2 = \vec{r} + \vec{r}_1$ gives

$$\vec{R} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{M} = \frac{m_1\vec{r}_1 + m_2(\vec{r} + \vec{r}_1)}{M} = \vec{r}_1 + \frac{m_2}{M}\vec{r} = \vec{r}_1 + \frac{m_2}{M}\vec{r} \ .$$

Thus we find

$$\vec{r}_1 = \vec{R} - \frac{m_2}{M}\vec{r}$$

and

$$\vec{r}_2 = \vec{r} + \vec{r}_1 = \vec{r} + \vec{R} - \frac{m_2}{M}\vec{r} = \vec{R} + \left(1 - \frac{m_2}{M}\right)\vec{r} = \vec{R} + \frac{m_1}{M}\vec{r} \; .$$

b) Well

$$\frac{\partial}{\partial x_i} = \frac{\partial X}{\partial x_i}\frac{\partial}{\partial X} + \frac{\partial x}{\partial x_i}\frac{\partial}{\partial x} = \frac{m_i}{M}\frac{\partial}{\partial X} \mp \frac{\partial}{\partial x} \; ,$$

and thus

$$\frac{\partial^2}{\partial x_i^2} = \left[\frac{m_i}{M}\right]^2 \frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial x^2} \mp 2\frac{m_i}{M}\frac{\partial}{\partial X}\frac{\partial}{\partial x} \; ,$$

where $i = 1$ for the upper case and $i = 2$ for the lower case. The other coordinate directions are treated identically *mutatis mutandis.* We then find that

$$-\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 = -\frac{\hbar^2}{2M}\nabla_{\text{cm}}^2 - \frac{\hbar^2}{2}\left(\frac{1}{m_1} + \frac{1}{m_2}\right)\nabla^2 = -\frac{\hbar^2}{2M}\nabla_{\text{cm}}^2 - \frac{\hbar^2}{2m}\nabla^2 \; ,$$

where define the reduced mass by

$$\frac{1}{m} = \frac{1}{m_1} + \frac{1}{m_2} \qquad \text{or} \qquad m = \frac{m_1 m_2}{m_1 + m_2} \; .$$

The symbol μ is often used for reduced mass, but μ has other uses as well (e.g., the magnetic moment). There are more quantities than symbols and at some point one has to start recycling.

Note

$$\frac{1}{m} \geq \frac{1}{m_i} \; ,$$

where i stands for 1 or 2 and equality only holds if the dropped mass is infinite. Thus

$$m \leq m_i \qquad \text{or} \qquad m \leq \min(m_1, m_2) \; .$$

If $m_1 = m_2$, then

$$m = \frac{m_1}{2} \; .$$

If $m_1/m_2 < 1$, then one can expand the reduced mass expression in the power series (e.g., Ar-238)

$$m = \frac{m_1}{1 + m_1/m_2} = m_1 \sum_k (-1)^k \left(\frac{m_1}{m_2}\right)^k \approx m_1 \left(1 - \frac{m_1}{m_2}\right) \; ,$$

where the last expression holds for $m_1/m_2 \ll 1$.

c) We make the anzatz that we can set

$$\psi_{\text{total}}(\vec{r}_1, \vec{r}_2) = \psi_{\text{cm}}(\vec{R})\psi(\vec{r}) \; .$$

The Schrödinger equation can then be written at once as

$$-\frac{\hbar^2}{2M}\frac{\nabla_{\text{cm}}^2 \psi_{\text{cm}}(\vec{R})}{\psi(\vec{R})} - \frac{\hbar^2}{2m}\frac{\nabla^2\psi(\vec{r})}{\psi(\vec{r})} + V(\vec{r}) + V_{\text{cm}}(\vec{R}) = E_{\text{total}} \; .$$

For the differential equation to hold for all $\vec{R}$ and $\vec{r}$, we must have

$$-\frac{\hbar^2}{2M}\frac{\nabla^2_{\mathrm{cm}}\psi_{\mathrm{cm}}(\vec{R})}{\psi(\vec{R})} + V_{\mathrm{cm}}(\vec{R}) = E_{\mathrm{cm}} \qquad \text{and} \qquad -\frac{\hbar^2}{2m}\frac{\nabla^2\psi(\vec{r})}{\psi(\vec{r})} + V(\vec{r}) = E \ ,$$

where E_{cm} and E are constants of separation that sum to E_{total}. We then have two 1-body Schrödinger equation problems:

$$\frac{\hbar^2}{2M}\nabla^2_{\mathrm{cm}}\psi_{\mathrm{cm}}(\vec{R}) + V_{\mathrm{cm}}(\vec{R})\psi(\vec{R}) = E_{\mathrm{cm}}\psi(\vec{R})$$

and

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r}) \ .$$

The center-of-mass problem is just the free particle Schrödinger equation if $V_{\mathrm{cm}}(\vec{R}) = 0$. In practice, it is probably impossible to have a potential that depends exactly on the center of mass. So $V_{\mathrm{cm}}(\vec{R})$ is likely only for the case, where the particles experience a slowly varying external potential $V_{\mathrm{ext}}(\vec{r}_1, \vec{r}_2)$ that can be approximated by $V_{\mathrm{ext}}(\vec{R}, \vec{R}) = V_{\mathrm{cm}}(\vec{R})$.

The relative problem is just the central force Schrödinger equation for one particle. The wave functions that solve the relative problem give the position of particle 2 relative to particle 1:

$$\psi(\vec{r}) = \psi_{21}(\vec{r}_2 - \vec{r}_1) \ .$$

Of course, one can get the wave function of particle 1 from particle 2 by using reversing the relative vector:

$$\psi(\vec{r}) = \psi_{21}(\vec{r}_2 - \vec{r}_1) = \psi_{21}[-(\vec{r}_1 - \vec{r}_2)] = \psi_{12}(\vec{r}_1 - \vec{r}_2)$$

or

$$\psi_{12}(\vec{r}_1 - \vec{r}_2) = \psi_{21}[-(\vec{r}_1 - \vec{r}_2)] \ .$$

The relative problem is not in an inertial frame, but it can be treated as if it were because it is a lawful equation derived from the Schrödinger equation. I always think that the reduced mass must account for the non-inertiality, but no textbook I know of spits out that notion directly.

The classical 2-body problem with only a central force separates in analogous way to the quantum 2-body problem. For example, the identical formula of the reduced mass appears.

Redaction: Jeffery, 2001jan01

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020 qfull 00200 1 3 0 easy math: electronic configurations to Ca

42. 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.

SUGGESTED ANSWER:

Ground State Electronic Configurations of Atoms from H to Ca

Atom	Electronic Configuration
H^1	$(1s)$
He^2	$(1s)^2$
Li^3	$(He)(2s)$
Be^4	$(He)(2s)^2$
B^5	$(He)(2s)^2(2p)$
C^6	$(He)(2s)^2(2p)^2$
N^7	$(He)(2s)^2(2p)^3$
O^8	$(He)(2s)^2(2p)^4$
F^9	$(He)(2s)^2(2p)^5$
Ne^{10}	$(He)(2s)^2(2p)^6$
Na^{11}	$(Ne)(3s)$
Mg^{12}	$(Ne)(3s)^2$
Al^{13}	$(Ne)(3s)^2(3p)$
Si^{14}	$(Ne)(3s)^2(3p)^2$
P^{15}	$(Ne)(3s)^2(3p)^3$
S^{16}	$(Ne)(3s)^2(3p)^4$
Cl^{17}	$(Ne)(3s)^2(3p)^5$
Ar^{18}	$(Ne)(3s)^2(3p)^6$
K^{19}	$(Ar)(4s)$
Ca^{20}	$(Ar)(4s)^2$

Redaction: Jeffery, 2008jan01

015 qfull 00190 2 5 0 tough thinking: 2nd order state correction

43. 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

$$|\psi_i^{(1)}\rangle = \sum_{\text{all } j,\ \text{except } j \neq i} c_{ij}^{(1)} |\psi_j^{(0)}\rangle = \sum_{\text{all } j,\ \text{except } j \neq i} \langle \psi_j^{(0)} | \psi_i^{(1)} \rangle |\psi_j^{(0)}\rangle$$

$$= \sum_{\text{all } j,\ \text{except } j \neq i} \frac{\langle \psi_j^{(0)} | H^{(1)} | \psi_i^{(0)} \rangle}{E_i^{(0)} - E_j^{(0)}} |\psi_j^{(0)}\rangle \ .$$

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

$$|\psi_i^{1\text{st}}\rangle = |\psi_i^{(0)}\rangle + \lambda|\psi_i^{(1)}\rangle \ ,$$

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 of 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.

SUGGESTED ANSWER:

a) Behold:

$$H^{(1)} | \psi_i^{(1)} \rangle + H^{(0)} | \psi_i^{(2)} \rangle = E_i^{(2)} | \psi_i^{(0)} \rangle + E_i^{(1)} | \psi_i^{(1)} \rangle + E_i^{(0)} | \psi_i^{(2)} \rangle \, .$$

b) Behold:

$$\langle \psi_i^{(0)} | H^{(1)} | \psi_i^{(1)} \rangle + \langle \psi_i^{(0)} | H^{(0)} | \psi_i^{(2)} \rangle = E_i^{(2)} \langle \psi_i^{(0)} | \psi_i^{(0)} \rangle + E_i^{(1)} \langle \psi_i^{(0)} | \psi_i^{(1)} \rangle + E_i^{(0)} \langle \psi_i^{(0)} | \psi_i^{(2)} \rangle$$

$$\langle \psi_i^{(0)} | H^{(1)} | \psi_i^{(1)} \rangle + E_i^{(0)} \langle \psi_i^{(0)} | \psi_i^{(2)} \rangle = E_i^{(2)} + 0 + E_i^{(0)} \langle \psi_i^{(0)} | \psi_i^{(2)} \rangle$$

$$E_i^{(2)} = \langle \psi_i^{(0)} | H^{(1)} | \psi_i^{(1)} \rangle$$

$$E_i^{(2)} = \langle \psi_i^{(0)} | H^{(1)} |$$

$$\left(\sum_{\text{all } j, \text{ except } j \neq i} \frac{\langle \psi_j^{(0)} | H^{(1)} | \psi_i^{(0)} \rangle}{E_i^{(0)} - E_j^{(0)}} | \psi_j^{(0)} \rangle \right)$$

$$E_i^{(2)} = \sum_{\text{all } j, \text{ except } j \neq i} \frac{|\langle \psi_j^{(0)} | H^{(1)} | \psi_i^{(0)} \rangle|^2}{E_i^{(0)} - E_j^{(0)}} \, .$$

c) Well now we take the inner product of the part (a) result with state $|\psi_j\rangle$ with $j \neq i$. Behold:

$$\langle \psi_j^{(0)} | H^{(1)} | \psi_i^{(1)} \rangle + \langle \psi_j^{(0)} | H^{(0)} | \psi_i^{(2)} \rangle = E_i^{(2)} \langle \psi_j^{(0)} | \psi_i^{(0)} \rangle + E_i^{(1)} \langle \psi_j^{(0)} | \psi_i^{(1)} \rangle + E_i^{(0)} \langle \psi_j^{(0)} | \psi_i^{(2)} \rangle$$

$$\langle \psi_j^{(0)} | H^{(1)} | \psi_i^{(1)} \rangle + E_j^{(0)} \langle \psi_j^{(0)} | \psi_i^{(2)} \rangle = 0 + E_i^{(1)} \langle \psi_j^{(0)} | \psi_i^{(1)} \rangle + E_i^{(0)} \langle \psi_j^{(0)} | \psi_i^{(2)} \rangle$$

$$\langle \psi_j^{(0)} | \psi_i^{(2)} \rangle = \left(\frac{1}{E_i^{(0)} - E_j^{(0)}} \right) \left(\langle \psi_j^{(0)} | H^{(1)} | \psi_i^{(1)} \rangle - E_i^{(1)} \langle \psi_j^{(0)} | \psi_i^{(1)} \rangle \right)$$

$$= \left(\frac{1}{E_i^{(0)} - E_j^{(0)}} \right) \left(\sum_{\text{all } k, \text{ except } k \neq i} \frac{\langle \psi_j^{(0)} | H^{(1)} | \psi_k^{(0)} \rangle \langle \psi_k^{(0)} | H^{(1)} | \psi_i^{(0)} \rangle}{E_i^{(0)} - E_k^{(0)}} \right.$$

$$\left. - \frac{E_i^{(1)} \langle \psi_j^{(0)} | H^{(1)} | \psi_i^{(0)} \rangle}{E_i^{(0)} - E_j^{(0)}} \right)$$

$$= \left(\frac{1}{E_i^{(0)} - E_j^{(0)}} \right) \left(\sum_{\text{all } k, \text{ except } k \neq i} \frac{\langle \psi_j^{(0)} | H^{(1)} | \psi_k^{(0)} \rangle \langle \psi_k^{(0)} | H^{(1)} | \psi_i^{(0)} \rangle}{E_i^{(0)} - E_k^{(0)}} \right.$$

$$\left. - \frac{\langle \psi_i^{(0)} | H^{(1)} | \psi_i^{(0)} \rangle \langle \psi_j^{(0)} | H^{(1)} | \psi_i^{(0)} \rangle}{E_i^{(0)} - E_j^{(0)}} \right) \, .$$

Note the coefficient is dimensionless as is required. Note also that if $j = i$, we get an undefined result—but, of course, $j \neq i$ by hypothesis.

d) For $n = 2$, the constraint specializes to

$$\langle \psi_i^{(2)} | \psi_i^{(0)} \rangle + \langle \psi_i^{(1)} | \psi_i^{(1)} \rangle + \langle \psi_i^{(0)} | \psi_i^{(2)} \rangle = 0 \ .$$

With

$$\langle \psi_i^{(0)} | \psi_i^{(k)} \rangle$$

pure real for all k, we find

$$\langle \psi_i^{(0)} | \psi_i^{(2)} \rangle = -\frac{1}{2} \langle \psi_i^{(1)} | \psi_i^{(1)} \rangle$$

$$= -\frac{1}{2} \left(\sum_{\text{all } j, \text{ except } j \neq i} \frac{\langle \psi_i^{(0)} | H^{(1)} | \psi_j^{(0)} \rangle}{E_i^{(0)} - E_j^{(0)}} \langle \psi_j^{(0)} | \right) \left(\sum_{\text{all } k, \text{ except } k \neq i} \frac{\langle \psi_k^{(0)} | H^{(1)} | \psi_i^{(0)} \rangle}{E_i^{(0)} - E_k^{(0)}} | \psi_k^{(0)} \rangle \right)$$

$$= -\frac{1}{2} \left(\sum_{\text{all } j, \text{ except } j \neq i} \frac{|\langle \psi_j^{(0)} | H^{(1)} | \psi_i^{(0)} \rangle|^2}{(E_i^{(0)} - E_j^{(0)})^2} \right) \ ,$$

Note the coefficient is dimensionless as is required.
Also note we made use of the fact that ket

$$|\psi\rangle = \sum_i c_i |i\rangle$$

has the corresponding bra

$$\langle \psi | = \sum_i c_i^* \langle i | \ .$$

This can be proven using general vector $|\alpha\rangle$. Behold:

$$\langle \alpha | \psi \rangle = \sum_i c_i \langle \alpha | i \rangle$$

$$\langle \psi | \alpha \rangle^* = \sum_i c_i \langle i | \alpha \rangle^*$$

$$\langle \psi | \alpha \rangle = \sum_i c_i^* \langle i | \alpha \rangle$$

$$\langle \psi | = \sum_i c_i^* \langle i | \ .$$

Redaction: Jeffery, 2008jan01

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	$= 0.8617 \times 10^{-6}\,\text{eV K}^{-1}$ $= 1.381 \times 10^{-16}\,\text{erg K}^{-1}$
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	$= 14.40\,\text{eV Å}$
Fine Structure constant	$\alpha = \dfrac{e^2}{\hbar c}$	$= 1/137.036$
Kinetic energy coefficient	$\dfrac{\hbar^2}{2m_e}$	$= 3.81\,\text{eV Å}^2$
	$\dfrac{\hbar^2}{m_e}$	$= 7.62\,\text{eV Å}^2$
Planck's constant	h	$= 4.15 \times 10^{-15}\,\text{eV}$
Planck's h-bar	$\hbar$	$= 6.58 \times 10^{-16}\,\text{eV}$
	hc	$= 12398.42\,\text{eV Å}$
	$\hbar c$	$= 1973.27\,\text{eV Å}$
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

$$H\Psi(x,t) = \left[\frac{p^2}{2m} + V(x)\right]\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

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

$$H\Psi(\vec{r}, t) = \left[\frac{p^2}{2m} + V(\vec{r})\right]\Psi(\vec{r}, t) = i\hbar\frac{\partial\Psi(\vec{r}, t)}{\partial t} \qquad H|\Psi\rangle = i\hbar\frac{\partial}{\partial t}|\Psi\rangle$$

$$H\psi(\vec{r}) = \left[\frac{p^2}{2m} + V(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r}) \qquad H|\psi\rangle = E|\psi\rangle$$

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

$$\text{General} \qquad \frac{d\langle A \rangle}{dt} = \left\langle \frac{\partial A}{\partial t} \right\rangle + \frac{1}{\hbar} \langle i[H(t), A] \rangle$$

$$\text{Ehrenfest's Theorem} \qquad \frac{d\langle \vec{r} \rangle}{dt} = \frac{1}{m} \langle \vec{p} \rangle \qquad \text{and} \qquad \frac{d\langle \vec{p} \rangle}{dt} = -\langle \nabla V(\vec{r}) \rangle$$

$$|\Psi(t)\rangle = \sum_j c_j(0) e^{-iE_j t/\hbar} |\phi_j\rangle$$

7 Simple Harmonic Oscillator (SHO) Formulae

$$V(x) = \frac{1}{2} m\omega^2 x^2 \qquad \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m\omega^2 x^2 \right) \psi = E\psi$$

$$\beta = \sqrt{\frac{m\omega}{\hbar}} \qquad \psi_n(x) = \frac{\beta^{1/2}}{\pi^{1/4}} \frac{1}{\sqrt{2^n n!}} H_n(\beta x) e^{-\beta^2 x^2/2} \qquad E_n = \left(n + \frac{1}{2} \right) \hbar\omega$$

$$H_0(\beta x) = H_0(\xi) = 1 \qquad H_1(\beta x) = H_1(\xi) = 2\xi$$
$$H_2(\beta x) = H_2(\xi) = 4\xi^2 - 2 \qquad H_3(\beta x) = H_3(\xi) = 8\xi^3 - 12\xi$$

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

$$\sigma_x \sigma_p = \Delta x \Delta p \geq \frac{\hbar}{2} \qquad \sigma_Q \sigma_Q = \Delta Q \Delta R \geq \frac{1}{2} |\langle i[Q,R] \rangle|$$

$$\sigma_H \Delta t_{\text{scale time}} = \Delta E \Delta t_{\text{scale time}} \geq \frac{\hbar}{2}$$

---

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

$$[J_i, J_j] = i\hbar\varepsilon_{ijk}J_k \qquad \text{(Einstein summation on } k\text{)} \qquad [J^2, \vec{J}] = 0$$

$$J^2|jm\rangle = j(j+1)\hbar^2|jm\rangle \qquad J_z|jm\rangle = m\hbar|jm\rangle$$

$$J_\pm = J_x \pm iJ_y \qquad J_\pm|jm\rangle = \hbar\sqrt{j(j+1) - m(m\pm1)}|jm\pm1\rangle$$

$$J_{\{\begin{smallmatrix}x\\y\end{smallmatrix}\}} = \left\{\begin{matrix}\frac{1}{2}\\\frac{1}{2i}\end{matrix}\right\}(J_+ \pm J_-) \qquad J_\pm^\dagger J_\pm = J_\mp J_\pm = J^2 - J_z(J_z \pm \hbar)$$

$$[J_{fi}, J_{gj}] = \delta_{fg}i\hbar\varepsilon_{ijk}J_k \qquad \vec{J} = \vec{J_1} + \vec{J_2} \qquad J^2 = J_1^2 + J_2^2 + J_{1+}J_{2-} + J_{1-}J_{2+} + 2J_{1z}J_{2z}$$

$$J_\pm = J_{1\pm} + J_{2\pm} \qquad |j_1 j_2 j m\rangle = \sum_{m_1 m_2, m=m_1+m_2} |j_1 j_2 m_1 m_2\rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m\rangle j_1 j_2 j m\rangle$$

$$|j_1 - j_2| \le j \le j_1 + j_2 \qquad \sum_{|j_1-j_2|}^{j_1+j_2} (2j+1) = (2j_1+1)(2j_2+1)$$

---

15 Spin 1/2 Formulae

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$|\pm\rangle_x = \frac{1}{\sqrt{2}} (|+\rangle \pm |-\rangle) \qquad |\pm\rangle_y = \frac{1}{\sqrt{2}} (|+\rangle \pm i|-\rangle) \qquad |\pm\rangle_z = |\pm\rangle$$

$$|++\rangle = |1,+\rangle|2,+\rangle \qquad |+-\rangle = \frac{1}{\sqrt{2}} (|1,+\rangle|2,-\rangle \pm |1,-\rangle|2,+\rangle) \qquad |--\rangle = |1,-\rangle|2,-\rangle$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_i \sigma_j = \delta_{ij} + i\varepsilon_{ijk}\sigma_k \qquad [\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k \qquad \{\sigma_i, \sigma_j\} = 2\delta_{ij}$$

$$(\vec{A} \cdot \vec{\sigma})(\vec{B} \cdot \vec{\sigma}) = \vec{A} \cdot \vec{B} + i(\vec{A} \times \vec{B}) \cdot \vec{\sigma}$$

$$\frac{d(\vec{S} \cdot \hat{n})}{d\alpha} = -\frac{i}{\hbar}[\vec{S} \cdot \hat{\alpha}, \vec{S} \cdot \hat{n}] \qquad \vec{S} \cdot \hat{n} = e^{-i\vec{S}\cdot\vec{\alpha}} \vec{S} \cdot \hat{n}_0 e^{i\vec{S}\cdot\vec{\alpha}} \qquad |\hat{n}_\pm\rangle = e^{-i\vec{S}\cdot\vec{\alpha}} |\hat{z}_\pm\rangle$$

$$e^{ixA} = \mathbf{1}\cos(x) + iA\sin(x) \quad \text{if } A^2 = \mathbf{1} \qquad e^{-i\vec{\sigma}\cdot\vec{\alpha}/2} = \mathbf{1}\cos(x) - i\vec{\sigma} \cdot \hat{\alpha}\sin(x)$$

$$\sigma_i f(\sigma_j) = f(\sigma_j)\sigma_i \delta_{ij} + f(-\sigma_j)\sigma_i(1 - \delta_{ij})$$

$$\mu_{\text{Bohr}} = \frac{e\hbar}{2m} = 0.927400915(23) \times 10^{-24}\,\text{J/T} = 5.7883817555(79) \times 10^{-5}\,\text{eV/T}$$

$$g = 2\left(1 + \frac{\alpha}{2\pi} + \dots\right) = 2.0023193043622(15)$$

$$\vec{\mu}_{\text{orbital}} = -\mu_{\text{Bohr}}\frac{\vec{L}}{\hbar} \qquad \vec{\mu}_{\text{spin}} = -g\mu_{\text{Bohr}}\frac{\vec{S}}{\hbar} \qquad \vec{\mu}_{\text{total}} = \vec{\mu}_{\text{orbital}} + \vec{\mu}_{\text{spin}} = -\mu_{\text{Bohr}}\frac{(\vec{L} + g\vec{S})}{\hbar}$$

$$H_\mu = -\vec{\mu} \cdot \vec{B} \qquad H_\mu = \mu_{\text{Bohr}}B_z\frac{(L_z + gS_z)}{\hbar}$$

16 Time-Independent Approximation Methods

$$H = H^{(0)} + \lambda H^{(1)} \qquad |\psi\rangle = N(\lambda)\sum_{k=0}^{\infty}\lambda^k|\psi_n^{(k)}\rangle$$

$$H^{(1)}|\psi_n^{(m-1)}\rangle(1 - \delta_{m,0}) + H^{(0)}|\psi_n^{(m)}\rangle = \sum_{\ell=0}^{m}E^{(m-\ell)}|\psi_n^{(\ell)}\rangle \qquad |\psi_n^{(\ell>0)}\rangle = \sum_{m=0,\ m\neq n}^{\infty}a_{nm}|\psi_n^{(0)}\rangle$$

$$|\psi_n^{\text{1st}}\rangle = |\psi_n^{(0)}\rangle + \lambda\sum_{\text{all }k,\ k\neq n}\frac{\left\langle\psi_k^{(0)}|H^{(1)}|\psi_n^{(0)}\right\rangle}{E_n^{(0)} - E_k^{(0)}}|\psi_k^{(0)}\rangle$$

$$E_n^{\text{1st}} = E_n^{(0)} + \lambda\left\langle\psi_n^{(0)}|H^{(1)}|\psi_n^{(0)}\right\rangle$$

$$E_n^{\text{2nd}} = E_n^{(0)} + \lambda\left\langle\psi_n^{(0)}|H^{(1)}|\psi_n^{(0)}\right\rangle + \lambda^2\sum_{\text{all }k,\ k\neq n}\frac{\left|\left\langle\psi_k^{(0)}|H^{(1)}|\psi_n^{(0)}\right\rangle\right|^2}{E_n^{(0)} - E_k^{(0)}}$$

$$E(\phi) = \frac{\langle\phi|H|\phi\rangle}{\langle\phi|\phi\rangle} \qquad \delta E(\phi) = 0$$

$$H_{kj} = \langle\phi_k|H|\phi_j\rangle \qquad H\vec{c} = E\vec{c}$$

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

$$[a_i, a_j^\dagger] = \delta_{ij} \qquad [a_i, a_j] = 0 \qquad [a_i^\dagger, a_j^\dagger] = 0 \qquad |N_1, \ldots, N_n\rangle = \frac{(a_n^\dagger)^{N_n}}{\sqrt{N_n!}}\cdots\frac{(a_1^\dagger)^{N_1}}{\sqrt{N_1!}}|0\rangle$$

$$\{a_i, a_j^\dagger\} = \delta_{ij} \qquad \{a_i, a_j\} = 0 \qquad \{a_i^\dagger, a_j^\dagger\} = 0 \qquad |N_1, \ldots, N_n\rangle = (a_n^\dagger)^{N_n}\cdots(a_1^\dagger)^{N_1}|0\rangle$$

$$\Psi_s(\vec{r})^\dagger = \sum_{\vec{p}} \frac{e^{-i\vec{p}\cdot\vec{r}}}{\sqrt{V}}a_{\vec{p}s}^\dagger \qquad \Psi_s(\vec{r}) = \sum_{\vec{p}} \frac{e^{i\vec{p}\cdot\vec{r}}}{\sqrt{V}}a_{\vec{p}s}$$

$$[\Psi_s(\vec{r}), \Psi_{s'}(\vec{r}\,')]_{\mp} = 0 \qquad [\Psi_s(\vec{r})^\dagger, \Psi_{s'}(\vec{r}\,')^\dagger]_{\mp} = 0 \qquad [\Psi_s(\vec{r}), \Psi_{s'}(\vec{r}\,')^\dagger]_{\mp} = \delta(\vec{r} - \vec{r}\,')\delta_{ss'}$$

$$|\vec{r}_1 s_1, \ldots, \vec{r}_n s_n\rangle = \frac{1}{\sqrt{n!}} \Psi_{s_n}(\vec{r}_n)^\dagger \ldots \Psi_{s_n}(\vec{r}_n)^\dagger |0\rangle$$

$$\Psi_s(\vec{r})^\dagger |\vec{r}_1 s_1, \ldots, \vec{r}_n s_n\rangle \sqrt{n+1} |\vec{r}_1 s_1, \ldots, \vec{r}_n s_n, \vec{r}s\rangle$$

$$|\Phi\rangle = \int d\vec{r}_1 \ldots d\vec{r}_n \, \Phi(\vec{r}_1, \ldots, \vec{r}_n) |\vec{r}_1 s_1, \ldots, \vec{r}_n s_n\rangle$$

$$1_n = \sum_{s_1 \ldots s_n} \int d\vec{r}_1 \ldots d\vec{r}_n \, |\vec{r}_1 s_1, \ldots, \vec{r}_n s_n\rangle\langle\vec{r}_1 s_1, \ldots, \vec{r}_n s_n| \qquad 1 = |0\rangle\langle 0| + \sum_{n=1}^{\infty} 1_n$$

$$N = \sum_{\vec{p}s} a_{\vec{p}s}^\dagger a_{\vec{p}s} \qquad T = \sum_{\vec{p}s} \frac{p^2}{2m} a_{\vec{p}s}^\dagger a_{\vec{p}s}$$

$$\rho_s(\vec{r}) = \Psi_s(\vec{r})^\dagger \Psi_s(\vec{r}) \qquad N = \sum_s \int d\vec{r} \, \rho_s(\vec{r}) \qquad T = \frac{1}{2m} \sum_s \int d\vec{r} \nabla \Psi_s(\vec{r})^\dagger \cdot \nabla \Psi_s(\vec{r})$$

$$\vec{j}_s(\vec{r}) = \frac{1}{2im} \left[\Psi_s(\vec{r})^\dagger \nabla \Psi_s(\vec{r}) - \Psi_s(\vec{r}) \nabla \Psi_s(\vec{r})^\dagger \right]$$

$$G_s(\vec{r} - \vec{r}\,') = \frac{3n}{2} \frac{\sin(x) - x\cos(x)}{x^3} \qquad g_{ss'}(\vec{r} - \vec{r}\,') = 1 - \delta_{ss'} \frac{G_s(\vec{r} - \vec{r}\,')^2}{(n/2)^2}$$

$$v_{2\text{nd}} = \frac{1}{2} \sum_{ss'} \int d\vec{r} d\vec{r}\,' \, v(\vec{r} - \vec{r}\,') \Psi_s(\vec{r})^\dagger \Psi_{s'}(\vec{r}\,')^\dagger \Psi_{s'}(\vec{r}\,') \Psi_s(\vec{r})$$

$$v_{2\text{nd}} = \frac{1}{2V} \sum_{pp'qq'} \sum_{ss'} v_{\vec{p}-\vec{p}\,'} \delta_{\vec{p}+\vec{q}, \vec{p}\,'+\vec{q}\,'} a_{\vec{p}s}^\dagger a_{\vec{q}s'}^\dagger a_{\vec{q}\,'s'} a_{\vec{p}\,'s} \qquad v_{\vec{p}-\vec{p}\,'} = \int d\vec{r} \, e^{-i(\vec{p}-\vec{p}\,')\cdot\vec{r}} v(\vec{r})$$

22 Klein-Gordon Equation

$$E = \sqrt{p^2c^2 + m^2c^4} \qquad \frac{1}{c^2}\left(i\hbar\frac{\partial}{\partial t}\right)^2 \Psi(\vec{r},t) = \left[\left(\frac{\hbar}{i}\nabla\right)^2 + m^2c^2\right]\Psi(\vec{r},t)$$

$$\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 + \left(\frac{mc}{\hbar}\right)^2\right]\Psi(\vec{r},t) = 0$$

$$\rho = \frac{i\hbar}{2mc^2}\left(\Psi^*\frac{\partial\Psi}{\partial t} - \Psi\frac{\partial\Psi^*}{\partial t}\right) \qquad \vec{j} = \frac{\hbar}{2im}\left(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\right)$$

$$\frac{1}{c^2}\left(i\hbar\frac{\partial}{\partial t} - e\Phi\right)^2 \Psi(\vec{r},t) = \left[\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}\right)^2 + m^2c^2\right]\Psi(\vec{r},t)$$

$$\Psi_+(\vec{p},E) = e^{i(\vec{p}\cdot\vec{r} - Et)/\hbar} \qquad \Psi_-(\vec{p},E) = e^{-i(\vec{p}\cdot\vec{r} - Et)/\hbar}$$