

Quantum Mechanics

NAME:

Homework 5: Multiple-Particle Systems, Identical Particles, and The Symmetrization Principle

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. Mathematically, 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

011 qmult 00210 1 1 3 easy memory: separation of variables 2

2. 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 :

$$\frac{\partial \text{LHS}}{\partial y} = 0 \quad \text{and} \quad \frac{\partial \text{LHS}}{\partial x} = \frac{\partial \text{RHS}}{\partial x} = 0 .$$

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 procedure. 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

011 qmult 00300 1 4 2 easy deducto-memory: relative/cm reduction

3. “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

011 qmult 00310 1 4 4 easy deducto-memory: reduced mass

4. 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) $m = \frac{1}{m_1 m_2}$. c) $m = \frac{m_1 + m_2}{m_1 m_2}$. d) $m = \frac{m_1 m_2}{m_1 + m_2}$. e) $m = \frac{1}{m_1}$.

SUGGESTED ANSWER: (d)

Wrong Answers:

- a) Dimensionally wrong.
- b) Dimensionally wrong.
- c) Dimensionally wrong.
- e) Dimensionally wrong and it only refers to one mass.

Redaction: Jeffery, 2001jan01

011 qmult 00400 1 4 2 easy deducto memory: spherical harmonics 1

5. 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

011 qmult 00420 1 4 3 easy deducto memory: spherical harmonic Y00

6. 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) $\frac{1}{\sqrt{4\pi}}$. 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: $m = 0, \pm 1, \pm 2, \dots, \pm \ell$.
- 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

$$a_0 = \frac{\hbar^2}{m_e [e^2 / (4\pi\epsilon_0)]} = \frac{\lambda_C}{2\pi} \frac{1}{\alpha} = 0.52917720859(36) \text{ \AA},$$

where e is the elementary charge, $\lambda_C = \hbar / (m_e c)$ is the Compton wavelength, and $\alpha \approx 1/137$ is the fine structure constant.

Redaction: Jeffery, 2001jan01

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

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

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

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.

Redaction: Jeffery, 2001jan01

011 qfull 00100 2 5 0 moderate thinking: 2-body reduced to 1-body problem

Extra keywords: (Gr-178:5.1)

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

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

If the V depends only on $\vec{r} = \vec{r}_2 - \vec{r}_1$ (the relative 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} .

- 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). 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 $V = V(\vec{r}) + V_{\text{cm}}(\vec{R})$. 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

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

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

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

where define the reduced mass by

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

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

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

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 ansatz 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

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

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

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

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

The relative problem is just the central force Schrödinger equation. 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:

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

or

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

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

9. 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 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 solutions: 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 those 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.

SUGGESTED ANSWER:

- a) The trial solution

$$\Phi = e^{\pm\kappa\phi}$$

obviously satisfies the differential equation. The general solution for a given κ^2 is then

$$\Phi = Ae^{\kappa\phi} + Be^{-\kappa\phi} ,$$

where A and B are undetermined constants.

We can see the value of parameterizing the constant of separation as κ^2 since it makes the solutions look nice.

In the special case of $\kappa^2 = 0$, we have

$$\Phi = A\phi + B ,$$

where A and B are undetermined constants.

Note that a 2nd order linear differential equation has only two independent solutions. So we have found all the linearly independent solutions for each κ^2 .

b) Well from the general solution for $\kappa \neq 0$, we get

$$Ae^{\kappa(\phi+2\pi)} + Be^{-\kappa(\phi+2\pi)} = Ae^{\kappa\phi} + Be^{-\kappa\phi}$$

and from its derivative,

$$\kappa Ae^{\kappa(\phi+2\pi)} - \kappa Be^{-\kappa(\phi+2\pi)} = \kappa Ae^{\kappa\phi} - \kappa Be^{-\kappa\phi} .$$

These equations can be rearranged to get

$$Ae^{\kappa\phi}(e^{2\pi\kappa} - 1) = -Be^{-\kappa\phi}(e^{-2\pi\kappa} - 1)$$

and

$$\kappa Ae^{\kappa\phi}(e^{2\pi\kappa} - 1) = \kappa Be^{-\kappa\phi}(e^{-2\pi\kappa} - 1)$$

or

$$Ae^{\kappa\phi}(e^{2\pi\kappa} - 1) = Be^{\kappa\phi}(e^{2\pi\kappa} - 1)$$

since $\kappa \neq 0$.

We now see that

$$Ae^{\kappa\phi}(e^{2\pi\kappa} - 1) = -Ae^{\kappa\phi}(e^{2\pi\kappa} - 1)$$

and

$$Be^{\kappa\phi}(e^{2\pi\kappa} - 1) = -Be^{\kappa\phi}(e^{2\pi\kappa} - 1) .$$

Since a number can only equal its additive inverse if it is zero, both of the last equations are $0 = 0$ equations. Say either of A or B is not zero, then we require

$$e^{2\pi\kappa} = 1 .$$

If both A and B are zero, there is no restriction on κ , but the solution is then not normalizable, and so not physical.

Say $\kappa = a + ib$, where a and b are pure real. Then

$$e^{2\pi a}[\cos(2\pi b) + i \sin(2\pi b)] = 1 ,$$

where we have used Euler's formula. We see that b must be an integer for the left-hand side to be pure real and positive. We then see that $a = 0$ for the equality to hold.

The conclusion is that κ must be an integer times i for a valid solution for $\kappa \neq 0$.

What if $\kappa = 0$? In this case, single-valuedness requires that $B = 0$. So

$$\Phi = A .$$

is the only valid solution for $\kappa = 0$.

c) Behold:

$$\Phi = e^{im\phi} ,$$

where $m = 0, \pm 1, \pm 2, \dots$

d) Well the eigenproblem is

$$L_z \Phi = \lambda \Phi$$

which is satisfied for solutions of the form

$$\Phi = e^{\kappa\phi}$$

with

$$\lambda = \frac{\hbar}{i}\kappa .$$

Now the boundary conditions (imposed by the single-valuedness condition) require that $\kappa = im$, where m is an integer. We know this from the part (b) answer. So the eigen states are

$$\Phi = e^{im\phi}$$

and the eigenvalues are

$$\lambda = m\hbar ,$$

where $m = 0, \pm 1, \pm 2, \dots$. The eigenvalues are pure real as required for those of an observable.

The eigen states for L_z are exactly the solutions to the azimuthal part of the Schrödinger equation that we obtained in the part (c) solution. We can now see that this is no surprize. If we operate on

$$L_z\Phi = m\hbar\Phi$$

with L_z , we get

$$\begin{aligned} L_z^2\Phi &= m^2\hbar^2\Phi \\ \frac{\hbar^2}{-1} \frac{d^2\Phi}{d\phi^2} &= m^2\hbar^2\Phi \\ \frac{d^2\Phi}{d\phi^2} &= -m^2\Phi \end{aligned}$$

which is just the the azimuthal angle part all over again. So the solutions to the eigenproblem for the z -component of angular momentum are the solutions to the azimuthal part. The azimuthal part is the really the eigenproblem

$$L_z^2\Phi = m^2\hbar^2\Phi$$

slightly disguised.

The m parameter is the z -component angular momentum quantum number or magnetic quantum number (MEL-59; ER-240). The latter name arises since the z -components of the angular momentum manifest themselves most noticeably in magnetic field phenomena.

e) By inspection, all the allowed normalized solutions are given by

$$\Phi = \frac{1}{\sqrt{2\pi}} e^{im\phi} .$$

In actual fact, one seldom normalizes the z -component of angular momentum solutions (AKA the azimuthal part solutions) when they stand alone. One normalizes the total angular squared solutions which are the spherical harmonics.

Redaction: Jeffery, 2001jan01

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

10. "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 (justified 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 quantum 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 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

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

is mathematically and, a priori, physically distinct 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 $\psi_{\text{com}}(\vec{r}_1 m_1, \vec{r}_2 m_2)$ be normalized. In quantum mechanics, $\psi_{\text{com}}(\vec{r}_1 m_1, \vec{r}_2 m_2)$ 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

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

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

019 qfull 00100 2 5 0 moderate thinking: permutation operator

11. 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

$$f(x_1, x_2) = x_1^3 x_2 .$$

But for a general proof, recall the definition of the derivative

$$\frac{df(x)}{dx} = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h} .$$

- d) Show that the permutation operation and the complex conjugation operation commute: i.e., show that

$$[Pf(x_1, x_2)]^* = P[f(x_1, x_2)^*] .$$

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.

SUGGESTED ANSWER:

- a) Say we evaluated $f(x_1, x_2)$ at specific point (a, b) . We'd get $f(a, b)$. Now

$$Pf(a, b) = f(b, a) .$$

So $Pf(x_1, x_2)$ has the same value at (a, b) that $f(x_1, x_2)$ as at (b, a) . A vector to (a, b) is mirrored in the $x_1 = x_2$ line by a vector to (b, a) . So we see that $Pf(x_1, x_2)$ is the mirror image of $f(x_1, x_2)$ in the $x_1 = x_2$ line.

- b) Well a proof by inspection enough—except for the paranoid, but anyway

$$P[f(x_1, x_2) + g(x_1, x_2)] = Ph(x_1, x_2) = h(x_2, x_1) = f(x_2, x_1) + g(x_2, x_1) = Pf(x_1, x_2) + Pg(x_1, x_2) ,$$

and thus

$$P[f(x_1, x_2) + g(x_1, x_2)] = Pf(x_1, x_2) + Pg(x_1, x_2) .$$

So P is indeed a linear operator.

- c) Well if

$$f(x_1, x_2) = x_1^3 x_2 ,$$

then

$$\frac{\partial f(x_1, x_2)}{\partial x_1} = 3x_1^2 x_2$$

and

$$P\left(\frac{\partial f(x_1, x_2)}{\partial x_1}\right) = P(3x_1^2 x_2) = 3x_2^2 x_1 = \frac{\partial f(x_2, x_1)}{\partial x_2} .$$

But to be general

$$P\left[\frac{\partial f(x_1, x_2)}{\partial x_1}\right] = P\left[\lim_{h \rightarrow 0} \frac{f(x_1 + h, x_2) - f(x_1, x_2)}{h}\right] = \lim_{h \rightarrow 0} \frac{f(x_2 + h, x_1) - f(x_2, x_1)}{h} = \frac{\partial f(x_2, x_1)}{\partial x_2} ,$$

where we have assumed by all that is righteous that we can commute P and the limit operation—all math would be absurd if we couldn't—and therefore we can. So, in general,

$$P \left[\frac{\partial f(x_1, x_2)}{\partial x_1} \right] = \frac{\partial f(x_2, x_1)}{\partial x_2} .$$

This result generalizes to all other permutation operators acting on functions with differentiating operators obviously.

d) Behold:

$$\begin{aligned} [Pf(x_1, x_2)]^* &= f(x_2, x_1)^* = f_{\text{Re}}(x_2, x_1) - if_{\text{Im}}(x_2, x_1) \\ &= Pf_{\text{Re}}(x_1, x_2) - iPf_{\text{Im}}(x_1, x_2) = P[f_{\text{Re}}(x_1, x_2) - if_{\text{Im}}(x_1, x_2)] \\ &= P[f(x_1, x_2)^*] \end{aligned}$$

which completes the proof.

Note we used the fact that the permutation operator is linear: i.e., that it distributes over addition. We proved this in the part (b) answer.

e) Behold:

$$\begin{aligned} \langle \phi | P | \psi \rangle &= \int_1 \int_2 \phi(x_1, x_2)^* P \psi(x_1, x_2) dx_2 dx_1 = \int_1 \int_2 \phi(x_1, x_2)^* \psi(x_2, x_1) dx_2 dx_1 \\ &= \int_2 \int_1 \phi(x_2, x_1)^* \psi(x_1, x_2) dx_1 dx_2 = \int_1 \int_2 \phi(x_2, x_1)^* \psi(x_1, x_2) dx_2 dx_1 \\ &= \left[\int_1 \int_2 \phi(x_2, x_1) \psi(x_1, x_2)^* dx_2 dx_1 \right]^* = \left[\int_1 \int_2 \psi(x_1, x_2)^* P \phi(x_1, x_2) dx_2 dx_1 \right]^* \\ &= \langle \psi | P | \phi \rangle^* , \end{aligned}$$

where we have used a transformation of the dummy variables and re-ordered the integrations. We see that $P = P^\dagger$ from the definition of a Hermitian conjugate. Thus P is guaranteed to have real eigenvalues and eigenfunctions that are orthogonal when there eigenvalues are distinct.

f) Assume $f(x_1, x_2)$ is an eigenfunction of P and λ is an eigenvalue which a priori could be complex. Then we find that

$$f(x_1, x_2) = P^2 f(x_1, x_2) = \lambda^2 f(x_1, x_2) .$$

Thus, $\lambda^2 = 1$. Thus, the only two eigenvalues are ± 1 . Note that they are real values as we knew from the part (e) answer.

Just to be tedious we can prove directly that $\lambda = \pm 1$ only. Note absolutely, positively, that $\lambda^2 = 1$, **NOT** $|\lambda|^2 = 1$ is the condition on λ . Let $\lambda = a + ib$. Now

$$\lambda^2 = a^2 - b^2 + 2iab = 1 .$$

Thus $a = 0$ or $b = 0$: they cannot both be zero and satisfy the equation. If $a = 0$, then we have a negative number equal to 1: this is a contradiction. Thus, we must have $b = 0$ and $a^2 = 1$. Since a is pure real by assumption $a = \pm 1$. Since $b = 0$, $\lambda = \pm 1$.

We could prove the result another way simpler way. Since $\lambda^2 = 1$ and we initially allow it to be complex, we must have

$$\lambda = \sqrt{1} = \sqrt{e^{i(\phi+2\pi n)}} ,$$

where $\phi = \tan^{-1}(y/x)$ (y is imaginary part and x is the real part) and n is any integer (Arf-300). The ϕ for 1 is zero. When we take the square root of $e^{i(\phi+2\pi n)}$, the only distinct values we get are for $n = 0$ and $n = 1$. Thus, we only get $\lambda = \pm 1$ and λ is pure real.

g) Well given $f(x_1, x_2)$, we can always form a function $f(x_2, x_1)$, and then the symmetrized functions

$$f_{\pm}(x_1, x_2) = \frac{1}{2} [f(x_1, x_2) \pm f(x_2, x_1)] ,$$

where the upper case is symmetric and the lower case antisymmetric. The symmetrized functions are obviously eigenfunctions of the permutation operator: the symmetric one has eigenvalue 1 and the antisymmetric one has eigenvalue -1 . Now

$$f(x_1, x_2) = f_+(x_1, x_2) + f_-(x_1, x_2) .$$

Thus, any function $f(x_1, x_2)$ can be expanded in eigenfunctions of the permutation operator. Thus, the eigenfunctions of the permutation operator constitute a complete set. A complete set with an uncountably infinite degeneracy since there are only two eigenvalues ± 1 . Since the permutation operator has a complete set for all functions, it has a complete for any two spatial dimension wave function space. Thus the permutation operator is formally a quantum mechanical observable for functions that are wave functions. Although, how one “observes” permutation is another story.

We can easily prove that a general symmetric and a general antisymmetric function are orthogonal. Orthogonality is, in fact, proven by the fact that these functions are eigen functions of the permutation operator and have distinct eigenvalues. But to be explicit, consider the inner product

$$\begin{aligned} \langle f_+ | f_- \rangle &= \int \int f_+(x_1, x_2)^* f_-(x_1, x_2) dx_1 dx_2 = - \int \int f_+(x_2, x_1)^* f_-(x_2, x_1) dx_1 dx_2 \\ &= - \int \int f_+(x_1, x_2)^* f_-(x_1, x_2) dx_1 dx_2 \\ &= - \langle f_+ | f_- \rangle , \end{aligned}$$

where we have used the symmetry properties and done a relabeling of the dummy indexes. We see that the inner product equals its own additive inverse, and therefore must be zero. So explicitly a general symmetric and a general antisymmetric function are orthogonal.

h) Well

$$PA(x_1, x_2)f(x_1, x_2) = A(x_2, x_1)f(x_2, x_1) = A(x_2, x_1)Pf(x_1, x_2)$$

if one can believe it. Since $A(x_1, x_2) \neq A(x_2, x_1)$ in general, P and $A(x_1, x_2)$ do not in general commute: i.e.,

$$[P, A(x_1, x_2)] \neq 0$$

in general. If $A(x_2, x_1) = A(x_1, x_2)$ (i.e., if $A(x_1, x_2)$ is symmetric), then P and $A(x_1, x_2)$ do commute: i.e.,

$$[P, A(x_1, x_2)] = 0$$

i) Since the particles are identical,

$$\begin{aligned} PH &= P \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_2^2} + V(x_1, x_2) \right] = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_2^2} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2} + V(x_2, x_1) \right] P \\ &= \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_2^2} + V(x_1, x_2) \right] P = HP , \end{aligned}$$

where we have used the fact that identical particles have identical mass and the fact that for identical particles $V(x_2, x_1) = V(x_1, x_2)$. So we have proven that P and H commute: i.e., that

$$[H, P] = 0 .$$

Given

$$H\psi(x_1, x_2) = E\psi(x_1, x_2) ,$$

it follows that

$$PH\psi(x_1, x_2) = HP\psi(x_1, x_2) = EP\psi(x_1, x_2) .$$

Thus $P\psi(x_1, x_2)$ is also an eigenstate of the Hamiltonian with the same energy as $\psi(x_1, x_2)$.

If $\psi(x_1, x_2)$ is not degenerate, then $P\psi(x_1, x_2)$ cannot be a physically distinct state: it can differ only by a global phase factor from $\psi(x_1, x_2)$. Thus

$$P\psi(x_1, x_2) = \psi(x_2, x_1) = e^{i\zeta}\psi(x_1, x_2) ,$$

where ζ is any phase. If we act with P again, we get

$$\psi(x_1, x_2) = e^{2i\zeta}\psi(x_1, x_2) .$$

This implies that $e^{2i\zeta} = 1$, and thus that the only allowed phases are 0 and π and the only allowed phase factors are ± 1 . Thus, non-energy-degenerate states are eigenstates of P as well as of H . This property often turns out to be useful in analyzing the possible wave functions of complex systems like molecules.

Note to be clear, a single non-degenerate state is either symmetric or antisymmetric. There are not two states of the same energy, one symmetric and one antisymmetric. If it were, it would violate our hypothesis of non-degeneracy in energy.

j) From the general time evolution formula

$$\frac{d\langle P \rangle}{dt} = \left\langle \frac{\partial P}{\partial t} \right\rangle + \frac{1}{\hbar} \langle i[H, P] \rangle = 0$$

since P has no explicit time dependence and commutes with H . Thus, P is a quantum mechanical constant of the motion as far as Schrödinger equation evolution goes. Therefore, states of definite symmetry retain that symmetry for all time as far as Schrödinger equation evolution goes.

But note if there is a perturbation Hamiltonian that does not commute with P , then symmetry can be lost or changed. Note also that I'm not sure what happens on wave function collapse which is a violation of Schrödinger equation evolution.

Redaction: Jeffery, 2001jan01

019 qfull 00200 1 3 0 easy math: symmetrization principle

12. 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

$$\Psi_{\text{mixed}} = c_i \Psi(\vec{r}_1 m_1, \vec{r}_2 m_2) + c_j \Psi(\vec{r}_2 m_2, \vec{r}_1 m_1) ,$$

where the only constraint on coefficients c_i and c_j is the the normalization constraint coefficients c_i and c_j

$$|c_i|^2 + |c_j|^2 + \text{Re}[c_i c_j \langle \Psi(\vec{r}_1 m_1, \vec{r}_2 m_2) | \Psi(\vec{r}_2 m_2, \vec{r}_1 m_1) \rangle] = 1 .$$

Note we are not assuming $\Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)$ and $P_{21} \Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)$ are orthogonal.

Argue that Ψ_{mixed} is physically distinct from $\Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)$ and $P_{21} \Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)$?

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 $\Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)$ and $P_{21} \Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)$ 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.

SUGGESTED ANSWER:

- a) In the first case, we have not obtained a new physical state. There is no physical distinction between wave functions that differ by a global phase factor.

In the second case, we have created a new physical state. The state $P_{2,1} \Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)$ is not the same as $\Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)$ and, to be clear, it will not evolve in general in the same way as $\Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)$ when subject to the same conditions. For example, say

$$\Psi(x_1, x_2) = C e^{-x_1^2/(2\sigma_a^2)} e^{-x_2^2/(2\sigma_b^2)} ,$$

where the wave function is a 1-dimensional Gaussian for both particles. If $\sigma_a \neq \sigma_b$, then clearly

$$P_{21} \Psi(x_1, x_2) = C e^{-x_2^2/(2\sigma_a^2)} e^{-x_1^2/(2\sigma_b^2)}$$

is physically distinct from $\Psi(x_1, x_2)$.

- b) We have not created a physically distinct state. There is no way to tell $P_{21} \Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)$ from $\Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)$. Furthermore both states will evolve identically when subject to the same conditions.

Note that for identical particles, the labels 1 and 2 are a formalism that works—well when the symmetrization principle is invoked. There is no way to actually distinguish the particles intrinsically. We can distinguish them dynamically if their spatial wave functions do not overlap or if they do overlap if they have non-overlapping spin states.

Mathematically the two states are different and distinct, of course, treating the coordinates as mathematically distinct dimensions. But this mathematical distinction can have no physical meaning.

c) In general,

$$\Psi_{\text{mixed}} = c_i \Psi(\vec{r}_1 m_1, \vec{r}_2 m_2) + c_j \Psi(\vec{r}_2 m_2, \vec{r}_1 m_1)$$

is clearly mathematically distinct from both $\Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)$ and $P_{21} \Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)$.

Given our assumptions, it is also physically distinct in general from $\Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)$ and $P_{21} \Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)$ which are physically indistinct as we argued in the part (b) answer. For example, for Ψ_{mixed} the probability density for particle 1 is

$$\begin{aligned} \rho(\vec{r}_1 m_1) &= \sum_{m_2} \int |\Psi_{\text{mixed}}|^2 d\vec{r}_2 \\ &= |c_i|^2 \sum_{m_2} \int |\Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)|^2 d\vec{r}_2 \\ &\quad + |c_j|^2 \sum_{m_2} \int |\Psi(\vec{r}_2 m_2, \vec{r}_1 m_1)|^2 d\vec{r}_2 \\ &\quad + 2\text{Re}[c_i c_j^* \sum_{m_2} \int \Psi(\vec{r}_1 m_1, \vec{r}_2 m_2) \Psi(\vec{r}_2 m_2, \vec{r}_1 m_1)^* d\vec{r}_2] \end{aligned}$$

is clearly different in general from the particle 1 probability density for $\Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)$: i.e., from

$$\rho(\vec{r}_1 m_1) = \sum_{m_2} \int |\Psi(\vec{r}_1 m_1, \vec{r}_2 m_2)|^2 d\vec{r}_2 .$$

Note that we have made use above of the identity

$$|a + b|^2 = |a|^2 + |b|^2 + \text{Re}(ab^*)$$

which is proven by

$$|a + b|^2 = |a|^2 + |b|^2 + a^* b + ab^* = |a|^2 + |b|^2 + (ab^*)^* + ab^* = |a|^2 + |b|^2 + \text{Re}(ab^*) .$$

The paradox of the degeneracy principle given the superposition interpretation of quantum mechanics is how can one create new physical states from a superposition of identical states. There are other paradoxes associated with the degeneracy principle (CT-1375–1377), but they seem a bit unfathomable to yours truly.

d) With only symmetrized states for identical particles (with only one kind of symmetrization for each type of identical particles), one cannot create physically distinct states by the linear combinations of versions of a symmetrized state with exchanges of any pair of particles. Note each of these versions is physically identical since the particles are identical and also mathematically identical (except for a change of sign in the case of antisymmetric states). One can choose one version to be the fiducial version arbitrarily. A linear combination is also now physically identical to all the versions. One can see this by exchanging pairs of particles (i.e., particle coordinates) in all terms in the linear combination until all particles are in the same slots in the wave function as in the fiducial version. Nothing happens on the exchanges if the particles are bosons and only sign changes happen on the exchanges if the particles are fermions. The linear combination then turns out to be just the fiducial version times a global phase factor which is physically meaningless.

To give an example consider the symmetrized state $\Psi(x_1, x_2, x_3)$. We now construct the linear combination

$$\Psi_{\text{mixed}} = c_i \Psi(x_1, x_2, x_3) + c_j \Psi(x_2, x_1, x_3) + c_k \Psi(x_2, x_3, x_1) .$$

By exchanges, we find

$$\begin{aligned}\Psi_{\text{mixed}} &= c_i\Psi(x_1, x_2, x_3) + c_j\Psi(x_2, x_1, x_3) + c_k\Psi(x_2, x_3, x_1) \\ &= c_i\Psi(x_1, x_2, x_3) \pm c_j\Psi(x_1, x_2, x_3) + (\pm 1)^2 c_k\Psi(x_1, x_2, x_3) \\ &= (c_i \pm c_j + c_k)\Psi(x_1, x_2, x_3) .\end{aligned}$$

Why can't we have the same type of particle having symmetric and antisymmetric states alternatively. Well then superposition of symmetric and antisymmetric states would be possible by ordinary quantum mechanics and those superpositions would not be symmetrized and we get the exchange degeneracy paradox all over again.

By the way the fact that integer-spin particles are bosons and half-integer-spin particles are fermions is proven by the spin-statistic theorem of quantum field theory. But this prove relies on hypotheses that themselves cannot be proven and may be wrong (CT-1387)—unless they have been proven since 1977. So taking nteger-spin particles are bosons and half-integer-spin particles are fermions can be regarded as an extra postulale or an extra part of the symmetrization principle.

- e) If the Hamiltonian is symmetric for the particles, then $[H, P_{ij}] = 0$ where i and j label any pair of the particles. From the general time evolution equation

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

(where Q is a general observable or actually an operator), we see that

$$\frac{d\langle P_{ij} \rangle}{dt} = 0$$

since the permutation operator has no intrinsic time dependence. In quantum mechancis jargon, the permutation operator is a constant of the motion. If a state starts out in an eigenstate of P_{ij} then it has $\langle P_{ij} \rangle = \pm 1$ initially and it will always have that eigenvalue. Thus, a state that starts out symmetric or antisymmetric stays that way as long as Schrödinger equation evolution occurs. This is consistent with the symmetrization principle. In fact, one could view it as a proof of the symmetrization principle if one takes it as an initial condition of the universe (in or out of time) that all identical particles type started out with symmetrized states.

However, this argument is invalid if wave function collapse actually happens since that violates Schrödinger equation evolution. Of course, wave function collapse doesn't happen in the many-worlds interpretation. It may be that if wave function collapse actually happens that the process (which we don't have a consensus theory) also conserves symmetrization.

- f) Yes, by the argument given above. But there is no rule that non-identical particles have to be in a symmetrized state. And if they are and an non-symmetric force starts to act then symmetrization will in general be lost.

If the Hamiltonian is symmetric, a common basis of energy eigenstates and symmetrized states can be found. But the basis states can be symmetric or antisymmetric and nothing forbids the state from being a mixed state that is not symmetrized.

An example, of non-identical particle system with a symmetric Hamiltonian is positronium neglecting any non-symmetry of the weak force of which I know nothing. Neglecting spin and other complications, the energy-eigenstates states (i.e., stationary states) are just those of the hydrogenic atom and are symmetrized. We find then

$$P_{2,1}\psi_{n\ell m}(\vec{r}_2 - \vec{r}_1) = P_{2,1}\psi_{n\ell m}(r, \theta, \phi) = \psi_{n\ell m}(r, \pi - \theta, \phi + \pi) = (-1)^\ell \psi_{n\ell m}(r, \theta, \phi) .$$

So both symmetric (even ℓ) and antisymmetric (odd ℓ) states occur. Thus, mixed states will in general not have definite symmetry.

- g) Say we have a state for a set of composite particles

$$\Psi(\dots, \{\vec{r}_i m_i\}, \dots, \{\vec{r}_j m_j\}, \dots) ,$$

where $\{r_i m_i\}$ is the set of coordinates for composite particle i 's constituent particles (which may be either fundamental or composites themselves) $\{r_j m_j\}$ is the set of coordinates for composite particle j 's constituent particles (which may be either fundamental or composites themselves). The state is symmetrized for the exchange of the constituent particles. and so is symmetric under the exchange of boson constituents and antisymmetric under the exchange of fermion constituents. Say we exchange composite particles i and j to create

$$\Psi(\dots, \{\vec{r}_j m_j\} \dots \{\vec{r}_i m_i\} \dots) = (-1)^n \Psi(\dots, \{\vec{r}_i m_i\} \dots \{\vec{r}_j m_j\} \dots) ,$$

where we have made use of the symmetrization and where n is number of fermions in a composite particle.

We see that the state is symmetrized for the exchange of composite particles. The composite particles are bosons if n is even and fermions if n is odd.

If the constituent particles are fundamental, we have proven the symmetrization principle for composite particles of fundamental particles. If the constituent particles are composites, we have proven the symmetrization principle for composite particles of composite particles.

h) Well for fermion state, we have

$$\Psi(\dots, \vec{r}_i m_i, \dots, \vec{r}_j m_j, \dots) ,$$

where the coordinates of particle i and j are label. If we try to create an new state by particle exchange, we find that

$$\Psi(\dots, \vec{r}_j m_j, \dots, \vec{r}_i m_i, \dots) = -\Psi(\dots, \vec{r}_i m_i, \dots, \vec{r}_j m_j, \dots)$$

since the original state was symmetrized. So the echange does not create a new state. But because the state is symmetrized, if $\vec{r}_i m_i = \vec{r}_j m_j = \vec{r}_{\text{pec}} m_{\text{pec}}$ (where ‘‘pec’’ stands for peculiar value),

$$\begin{aligned} & \Psi(\dots, \vec{r}_j m_j = \vec{r}_{\text{pec}} m_{\text{pec}}, \dots, \vec{r}_i m_i = \vec{r}_{\text{pec}} m_{\text{pec}}, \dots) \\ &= -\Psi(\dots, \vec{r}_i m_i = \vec{r}_{\text{pec}} m_{\text{pec}}, \dots, \vec{r}_j m_j = \vec{r}_{\text{pec}} m_{\text{pec}}, \dots) , \end{aligned}$$

The only way number can equal its own additive inverse is if the number is zero. So a properly symmetrized wave function for fundamental fermions gives zero probability amplitude for two particles at the same space coordinate and same spin coordinate.

Because the wave function is continuous in reality, we expect relatively low probability amplitude for two particles near the same space coordinate and at the same spin coordinate.

What if the fermions are composites is there still a spatial-spin Pauli exclusion principle? This seems to be an unspeakable in quantum mechanics—an obvious point that no one discusses. But I imagine yes. Say two composite fermions

Redaction: Jeffery, 2008jan01

019 qfull 02000 2 5 0 moderate thinking: symmetrization of 4 orthonormal single-particle states

13. 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),

$$\begin{aligned} \langle 12|12\rangle &= \left[\int \psi_a(x_1)^* \psi_a(x_1) dx_1 (c_{a+}^* \quad c_{a-}^*)_1 \begin{pmatrix} c_{a+} \\ c_{a-} \end{pmatrix}_1 \right] \\ &\quad \times \left[\int \psi_b(x_2)^* \psi_b(x_2) dx_2 (c_{b+}^* \quad c_{b-}^*)_2 \begin{pmatrix} c_{b+} \\ c_{b-} \end{pmatrix}_2 \right] . \end{aligned}$$

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 simplest and most obvious normalized 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 if $a = b$ for fermions?

SUGGESTED ANSWER:

a) Behold:

$$|12\rangle = |a1\rangle|b2\rangle \quad \text{and} \quad |21\rangle = |a2\rangle|b1\rangle$$

which are just the allowed product states. More complicated states can be constructed if the particles are in mixtures of the two states just given. If $a = b$, then one can construct only one state

$$|12\rangle = |a1\rangle|a2\rangle .$$

b) Behold:

$$|12\rangle = \frac{1}{\sqrt{2(1 + \delta_{ab})}} (|a1\rangle|b2\rangle \pm |a2\rangle|b1\rangle) ,$$

where the upper case is for bosons and the lower case is for fermions.

I don't think there are any other possible physical states that can be constructed. There are only two possible product states. And only a symmetrized mixed state is allowed.

The Kronecker delta allows for the case that $a = b$ for bosons. Obviously, we never had to symmetrize at all for bosons if $a = b$. If $a = b$ for fermions, the state is null, and thus no physical state can be constructed in this case. The nullness is a manifestation of the Pauli exclusion principle (a corollary of the symmetrization postulate): two fermions cannot be in found in the same single-particle state (as specified by a C.S.C.O.: i.e., a complete set of commuting observables (CT-143)). "Cannot be found" has to be interpreted as the probability for two fermions in the same single-particle state is zero or that the probability of collapsing the wave function to having two fermions in the same single-particle state is zero. So if $a = b$ for fermions, then a physical symmetrized state cannot be created from product states.

Redaction: Jeffery, 2001jan01

019 qfull 02100 1 5 0 easy thinking: slater determinant, triplet singlet

Extra keywords: (Gr-181:5.3)

14. Say that we have obtained four distinct orthonormal single-particle eigenstates for identical spin 1/2 particles:

$$\psi_a(\vec{r})\chi_+ , \quad \psi_a(\vec{r})\chi_- , \quad \psi_b(\vec{r})\chi_+ , \quad \psi_b(\vec{r})\chi_- ,$$

where the spinors are

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix} .$$

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.,

$$\psi_a(\vec{r}_1)\chi_{+,1}\psi_a(\vec{r}_2)\chi_{-,1} \quad \text{and} \quad \psi_a(\vec{r}_2)\chi_{+,2}\psi_a(\vec{r}_1)\chi_{-,2}$$

are the same product state for identical particles. Write down the product states. Are the product states orthonormal? 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 symmetrized states of the part (d) answer to be stationary states and when you would expect the triplet-singlet set of symmetrized states to be stationary states.

SUGGESTED ANSWER:

- a) Well the Pauli exclusion principle means that we have no replacement in the choice: we can't put two identical particles into the same state. The order of selection of a pair does not result in a distinct product state. The right counting procedure is to use the binomial coefficient rule:

$$\binom{n}{k} = \binom{4}{2} = \frac{4!}{2!2!} = 6 .$$

The possible product states are

$$\begin{aligned} \psi_a(\vec{r}_1)\chi_{+,1}\psi_a(\vec{r}_2)\chi_{-,2} , & \quad \psi_a(\vec{r}_1)\chi_{+,1}\psi_b(\vec{r}_2)\chi_{+,2} , & \quad \psi_a(\vec{r}_1)\chi_{+,1}\psi_b(\vec{r}_2)\chi_{-,2} , \\ \psi_a(\vec{r}_1)\chi_{-,1}\psi_b(\vec{r}_2)\chi_{+,2} , & \quad \psi_a(\vec{r}_1)\chi_{-,1}\psi_b(\vec{r}_2)\chi_{-,2} , & \quad \psi_b(\vec{r}_1)\chi_{+,1}\psi_b(\vec{r}_2)\chi_{-,2} . \end{aligned}$$

The product states are obviously normalized: e.g.,

$$\begin{aligned} \int |\psi_a(\vec{r}_1)\chi_{+,1}\psi_a(\vec{r}_2)\chi_{-,2}|^2 d\vec{r}_1 d\vec{r}_2 &= \int |\psi_a(\vec{r}_1)|^2 d\vec{r}_1 \times \int |\psi_a(\vec{r}_2)|^2 d\vec{r}_2 \times \chi_{+,1}^\dagger \chi_{+,1} \times \chi_{-,2}^\dagger \chi_{-,2} \\ &= 1 \times 1 \times 1 \times 1 = 1 . \end{aligned}$$

Are the product states orthogonal? Since there are the distinct product states of orthogonal single-particle states, the answer is yes. Any two product states must have different be single-particle states for at least one particle in order to be distinct product states. Those different single-particle states will lead to a zero for the inner product of the states.

If the particles were distinct, exchanging the labels would create different two-particle product states. From another perspective order would matter in the counting of states: for example, the first chosen state would be given to particle 1 and the second to particle 2. One would count the states by

$$\frac{n!}{k!} = \frac{4!}{2!} = 12 .$$

Thus, there are 12 product states for distinct particles.

One constructs a symmetrized state from a product state by forming a sum of all permutations of the particle labels with odd permutations getting a negative sign. Since there are 6 distinct product states for identical particles, there are 6 distinct linearly-independent symmetrized states too. Obviously, one can create infinitely many linear combinations of these states.

- b) The answer is yes. Let's consider normalization first. Consider a symmetrized state in which constructed from products of single-particle states. For N particles, the normalization factor of the symmetrized state is $1/\sqrt{N!}$. When the symmetrized state is inner-producted with itself

there are $(N!)^2$ terms to be fully integrated/summed over. The direct terms each give 1 for $N!$ which is canceled by the normalization factor squared, and so one gets 1 overall. The cross terms are all zero since for at least one particle label, there must be two distinct orthogonal single-particle states being inner-producted with each other and the single-particle states are all orthogonal by assumption. The construction of the symmetrized state guarantees this. The construction is a bit trickier conceptually for bosons than for fermions since there is no Pauli exclusion principle to forbid the multiple occupation of single-particle states.

What of orthogonality? Well different symmetrized states, must differ in at least 1 single-particle state that went into their construction. Thus, in every term in the inner product of one symmetrized state with another, there must be at least one single-particle inner product of orthogonal states. Thus every term is zero and the overall inner product is zero.

c) Behold:

$$\frac{1}{\sqrt{2}} \det \begin{vmatrix} \psi_a(\vec{r}_1)\chi_{+,1} & \psi_a(\vec{r}_1)\chi_{-,1} \\ \psi_a(\vec{r}_2)\chi_{+,2} & \psi_a(\vec{r}_2)\chi_{-,2} \end{vmatrix} = \psi_a(\vec{r}_1)\psi_a(\vec{r}_2) \frac{1}{\sqrt{2}} [\chi_{+,1}\chi_{-,2} - \chi_{+,2}\chi_{-,1}]$$

and

$$\frac{1}{\sqrt{2}} \det \begin{vmatrix} \psi_b(\vec{r}_1)\chi_{+,1} & \psi_b(\vec{r}_1)\chi_{-,1} \\ \psi_b(\vec{r}_2)\chi_{+,2} & \psi_b(\vec{r}_2)\chi_{-,2} \end{vmatrix} = \psi_b(\vec{r}_1)\psi_b(\vec{r}_2) \frac{1}{\sqrt{2}} [\chi_{+,1}\chi_{-,2} - \chi_{+,2}\chi_{-,1}] .$$

Both of these states are spin 1/2 singlet states. Since the single-particle spatial states are the same the space part of the state is symmetric, and so the spin part must be antisymmetric in order for the overall state to be antisymmetric. Thus, only singlet spin states are possible.

d) Well this is tedious. Behold:

$$\begin{aligned} \frac{1}{\sqrt{2}} \det \begin{vmatrix} \psi_a(\vec{r}_1)\chi_{+,1} & \psi_b(\vec{r}_1)\chi_{+,1} \\ \psi_a(\vec{r}_2)\chi_{+,2} & \psi_b(\vec{r}_2)\chi_{+,2} \end{vmatrix} &= \frac{1}{\sqrt{2}} [\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) - \psi_a(\vec{r}_2)\psi_b(\vec{r}_1)]\chi_{+,1}\chi_{+,2} , \\ \frac{1}{\sqrt{2}} \det \begin{vmatrix} \psi_a(\vec{r}_1)\chi_{+,1} & \psi_b(\vec{r}_1)\chi_{-,1} \\ \psi_a(\vec{r}_2)\chi_{+,2} & \psi_b(\vec{r}_2)\chi_{-,2} \end{vmatrix} &= \frac{1}{\sqrt{2}} [\psi_a(\vec{r}_1)\chi_{+,1}\psi_b(\vec{r}_2)\chi_{-,2} - \psi_a(\vec{r}_2)\chi_{+,2}\psi_b(\vec{r}_1)\chi_{-,1}] \\ &= \frac{1}{\sqrt{2}} [\psi_a(\vec{r}_1)\psi_b(\vec{r}_2)\chi_{+,1}\chi_{-,2} - \psi_a(\vec{r}_2)\psi_b(\vec{r}_1)\chi_{+,2}\chi_{-,1}] \\ \frac{1}{\sqrt{2}} \det \begin{vmatrix} \psi_a(\vec{r}_1)\chi_{-,1} & \psi_b(\vec{r}_1)\chi_{+,1} \\ \psi_a(\vec{r}_2)\chi_{-,2} & \psi_b(\vec{r}_2)\chi_{+,2} \end{vmatrix} &= \frac{1}{\sqrt{2}} [\psi_a(\vec{r}_1)\chi_{-,1}\psi_b(\vec{r}_2)\chi_{+,2} - \psi_a(\vec{r}_2)\chi_{-,2}\psi_b(\vec{r}_1)\chi_{+,1}] \\ &= \frac{1}{\sqrt{2}} [\psi_a(\vec{r}_1)\psi_b(\vec{r}_2)\chi_{-,1}\chi_{+,2} - \psi_a(\vec{r}_2)\psi_b(\vec{r}_1)\chi_{-,2}\chi_{+,1}] \\ \frac{1}{\sqrt{2}} \det \begin{vmatrix} \psi_a(\vec{r}_1)\chi_{-,1} & \psi_b(\vec{r}_1)\chi_{-,1} \\ \psi_a(\vec{r}_2)\chi_{-,2} & \psi_b(\vec{r}_2)\chi_{-,2} \end{vmatrix} &= \frac{1}{\sqrt{2}} [\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) - \psi_a(\vec{r}_2)\psi_b(\vec{r}_1)]\chi_{-,1}\chi_{-,2} , \end{aligned}$$

The middle two symmetrized states may look the same at first glance, but they are distinct. The first has the ψ_a and χ_+ states together for one particle label and the ψ_b and χ_- states together for other particle label. The second has the ψ_a and χ_- states together for one particle label and the ψ_b and χ_+ states together for other particle label.

The first and last symmetrized states are $m = 1$ and $m = -1$ states of the spin triplet. The middle two symmetrized states are not triplet or singlet states and have not special name known to yours truly.

e) Ennui, ennui. OK, let's add/subtract the middle two symmetrized states from the part (d) answer with another normalization factor of $1/\sqrt{2}$ to get

$$\begin{aligned} \psi_{\pm} &= \frac{1}{2} \{ [\psi_a(\vec{r}_1)\psi_b(\vec{r}_2)\chi_{+,1}\chi_{-,2} - \psi_a(\vec{r}_2)\psi_b(\vec{r}_1)\chi_{+,2}\chi_{-,1}] \pm [\psi_a(\vec{r}_1)\psi_b(\vec{r}_2)\chi_{-,1}\chi_{+,2} - \psi_a(\vec{r}_2)\psi_b(\vec{r}_1)\chi_{-,2}\chi_{+,1}] \} \\ &= \frac{1}{2} \{ \psi_a(\vec{r}_1)\psi_b(\vec{r}_2)[\chi_{+,1}\chi_{-,2} \pm \chi_{-,1}\chi_{+,2}] - \psi_a(\vec{r}_2)\psi_b(\vec{r}_1)[\chi_{-,1}\chi_{+,2} \pm \chi_{-,2}\chi_{+,1}] \} \\ &= \frac{1}{2} \{ \psi_a(\vec{r}_1)\psi_b(\vec{r}_2)[\chi_{+,1}\chi_{-,2} \pm \chi_{-,1}\chi_{+,2}] - \psi_a(\vec{r}_2)\psi_b(\vec{r}_1)[\chi_{-,1}\chi_{+,2} \pm \chi_{+,1}\chi_{-,2}] \} \\ &= \frac{1}{2} [\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) \mp \psi_a(\vec{r}_2)\psi_b(\vec{r}_1)] [\chi_{+,1}\chi_{-,2} \pm \chi_{-,1}\chi_{+,2}] \\ &= \frac{1}{\sqrt{2}} [\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) \mp \psi_a(\vec{r}_2)\psi_b(\vec{r}_1)] \frac{1}{\sqrt{2}} [\chi_{+,1}\chi_{-,2} \pm \chi_{-,1}\chi_{+,2}] . \end{aligned}$$

The upper case solution is spatially antisymmetric and spin symmetric, and thus is a triplet state with $s = 1$ and $m = 0$. The lower case solution is spatially symmetric and spin antisymmetric, and thus is a singlet state with $s = 0$ and $m = 0$.

The first and last symmetrized states from the part (d) answer and the two symmetrized states constructed in this answer constitute a full triplet-singlet set of states.

- e) Well the part (d) set would be the stationary states if single particle states had a strong spatial-spin coupling and there was no spin-spin coupling at all (i.e., no interaction between the spins of the particles). For example, in this case the energies of

$$\psi_a(\vec{r})\chi_+ \quad \text{and} \quad \psi_a(\vec{r})\chi_-$$

would be different because strong spatial-spin coupling.

On the other hand, if there were no spatial-spin coupling, but a there was a spin-spin interaction, then the triplet (parallel spins) and singlet (anti-parallel spins) would have different eigen-energies. If there were an external force which acted on the spins, the degeneracy of the triplet states would be broken and they would have different eigen-energies.

Now what the devil you ask if there were no spatial-spin coupling and no spin-spin coupling? In this case, spin has no affect on energy. Well first off this is unlikely if the particles are actually close enough together to require symmetrized states. But as an idealized limit, what does one expect? Well both sets of states are equivalent stationary states then and they would all be degenerate since the single-particle state occupation number is 1 for each single-particle state. You would probably, then find the system in some mixed state relative to both sets of stationary states and this mixed state was set by past history.

Actually, the most likely case is that you have both spatial-spin coupling and spin-spin coupling to some degree or other. This is actually the most likely case. It's true for real atoms. Then to be exact neither set of states are likely to be stationary states. If one or other of the couplings is dominant, then the corresponding set of stationary states are probably a good approximation. If neither is dominant, then you'd have to solve for the stationary states. How would this be done? Well there are ways. The most usual one is to assemble a complete set of states for the system (not just the 4 states in the two sets we've considered) and diagonalize the true Hamiltonian matrix assembled from the complete set. This would be usually be a very large computation that would be done on a computer.

Redaction: Jeffery, 2001jan01

019 qfull 02200 3 5 0 tough thinking: 2-particle infinite square well

Extra keywords: (Gr-182:5.4)

15. The set of individual eigen states for a 1-dimensional, infinite square well confined to $[0, a]$ can be written $|n\rangle$ where $n = 1, 2, 3, \dots$. 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 identified 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

$$|a1, b1\rangle = |a1\rangle|b1\rangle \quad \text{with} \quad E_{\text{red}} = 2 .$$

SUGGESTED ANSWER:

- a) The 2-particle Schrödinger equation for the infinite square well confined to $[0, a]$ is

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x_a^2} + \frac{\partial^2}{\partial x_b^2} \right) \psi = E\psi ,$$

where indexes a and b label the particles. It's poor choice to use a and b since a is also the infinite well width.

- b) The code is given further below. The table of energy levels follows here.

Table of Energy Levels

Level No.	n_1	n_2	n_1^2	n_2^2	E_{red}	Non-Identical Particle Degeneracy	Identical Boson Degeneracy	Identical Fermions Degeneracy
1	1	1	1	1	2	1	1	0
2	1	2	1	4	5	2	1	1
3	2	2	4	4	8	1	1	0
4	1	3	1	9	10	2	1	1
5	2	3	4	9	13	2	1	1
6	1	4	1	16	17	2	1	1
7	3	3	9	9	18	1	1	0
8	2	4	4	16	20	2	1	1
9	3	4	9	16	25	2	1	1
10	1	5	1	25	26	2	1	1
11	2	5	4	25	29	2	1	1
12	4	4	16	16	32	1	1	0
13	3	5	9	25	34	2	1	1
14	1	6	1	36	37	2	1	1
15	2	6	4	36	40	2	1	1
16	4	5	16	25	41	2	1	1
17	3	6	9	36	45	2	1	1
18	1	7	1	49	50	2	1	1
19	5	5	25	25	50	1	1	0

Note—For non-identical particles interchanging the distinct values of n_1 and n_2 creates a different state, but it's too tedious to write those out explicitly. We merely note that those cases exist and the energy level has a degeneracy of 2 as indicated in the table. For identical particles interchanging the values of n_1 and n_2 does not create a different state. Thus for bosons the degeneracy is always 1 for each energy level. For fermions, if $n_1 = n_2$ no state is allowed by the Pauli exclusion principle and the degeneracy is zero. Note that there are two energy levels counted with reduced energy 50. Of course, there is actually only one energy level of reduced energy 50. This is the lowest energy example of can be called an accidental degeneracy. For each case one should just add the degeneracies: i.e., 3 for non-identical particles, 2 for identical bosons, and 1 for identical fermions. Computationally it's tricky to explicitly handle accidental degeneracies, and so we haven't done so.

- c) For non-identical particles,

$$\begin{aligned} |a1, b1\rangle &= |a1\rangle|b1\rangle & E_{\text{red}} &= 2 , \\ |a1, b2\rangle &= |a1\rangle|b2\rangle & E_{\text{red}} &= 5 , \\ |a2, b1\rangle &= |a2\rangle|b1\rangle & E_{\text{red}} &= 5 , \\ |a2, b2\rangle &= |a2\rangle|b2\rangle & E_{\text{red}} &= 8 , \\ |a1, b3\rangle &= |a1\rangle|b3\rangle & E_{\text{red}} &= 10 , \\ |a3, b1\rangle &= |a3\rangle|b1\rangle & E_{\text{red}} &= 10 . \end{aligned}$$

For bosons,

$$\begin{aligned}
 |1, 1\rangle &= |a1\rangle|b1\rangle & E_{\text{red}} &= 2, \\
 |1, 2\rangle &= \frac{1}{\sqrt{2}} (|a1\rangle|b2\rangle + |b1\rangle|a2\rangle) & E_{\text{red}} &= 5, \\
 |2, 2\rangle &= |2\rangle|2\rangle & E_{\text{red}} &= 8, \\
 |1, 3\rangle &= \frac{1}{\sqrt{2}} (|a1\rangle|b3\rangle + |b1\rangle|a3\rangle) & E_{\text{red}} &= 10.
 \end{aligned}$$

For fermions,

$$\begin{aligned}
 |1, 2\rangle &= \frac{1}{\sqrt{2}} (|a1\rangle|b2\rangle - |b1\rangle|a2\rangle) & E_{\text{red}} &= 5, \\
 |1, 3\rangle &= \frac{1}{\sqrt{2}} (|a1\rangle|b3\rangle - |b1\rangle|a3\rangle) & E_{\text{red}} &= 10, \\
 |2, 3\rangle &= \frac{1}{\sqrt{2}} (|a2\rangle|b3\rangle - |b2\rangle|a3\rangle) & E_{\text{red}} &= 13, \\
 |1, 4\rangle &= \frac{1}{\sqrt{2}} (|a1\rangle|b4\rangle - |b1\rangle|a4\rangle) & E_{\text{red}} &= 17.
 \end{aligned}$$

Fortran Code

```

      print*
      print*, 'Cute, but I don''t see any simple ',
      &      'generalization to n-tuples.'
      print*
      nsqmax=50
      ilevel=0
      do nsq=1,nsqmax
      do n1=1,nsq
      if(n1**2 .gt. nsq/2) go to 110
      * Note if n1**2 .gt. nsq/2, then since n1**2 is integer, n1**2 must
      * be greater than nsq/2+1/2 for nsq non-integer.
      idif=nsq-n1**2
      n2a=int(sqrt(real(idif)))
      n2b=n2a+1
      n2=0
      if(n2a**2 .eq. idif) n2=n2a
      if(n2b**2 .eq. idif) n2=n2b
      if(n2**2 .eq. idif) then
      ilevel=ilevel+1
      if(n1 .ne. n2) then
      ndeg=2
      ndegf=1
      else
      ndeg=1
      ndegf=0
      end if
      print920,ilevel,n1,n2,n1**2,n2**2,nsq,ndeg,1,ndegf
920    format(1x,i5,2x,8('&',i5,2x),' \\cr')
      end if
      end do
110  continue
      end do

```

Redaction: Jeffery, 2001jan01

16. 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:

$$|1, 2\rangle = \frac{1}{\sqrt{2(1 + \delta_{ab})}} (|a1, b2\rangle \pm |a2, b1\rangle) ,$$

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**

$$|1, 2\rangle = \frac{1}{\sqrt{2(1 + \delta_{ab})}} (|a1, b2\rangle \pm |a2, b1\rangle) ,$$

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.

SUGGESTED ANSWER:

a) Behold:

$$\langle \Delta x^2 \rangle = \langle (x_1 - x_2)^2 \rangle = \langle x_1^2 \rangle + \langle x_2^2 \rangle - 2\langle x_1 x_2 \rangle .$$

b) For distinct particles,

$$\begin{aligned} \langle x_1^2 \rangle &= \langle a1, b2|x_1^2|a1, b2\rangle = \langle a1|x_1^2|a1\rangle\langle b2|b2\rangle = \langle x^2 \rangle_a , \\ \langle x_2^2 \rangle &= \langle a1, b2|x_2^2|a1, b2\rangle = \langle a1|a1\rangle\langle b2|x_2^2|b2\rangle = \langle x^2 \rangle_b , \\ \langle x_1 x_2 \rangle &= \langle a1, b2|x_1 x_2|a1, b2\rangle = \langle a1|x_1|a1\rangle\langle b2|x_2|b2\rangle = \langle x \rangle_a \langle x \rangle_b , \end{aligned}$$

where the particle labels 1 and 2 are irrelevant to the single-particle state expectation values, and so we have dropped them. Thus,

$$\langle \Delta x^2 \rangle = \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2\langle x \rangle_a \langle x \rangle_b ,$$

In the case that $|a\rangle = |b\rangle$,

$$\langle \Delta x^2 \rangle = 2\langle x^2 \rangle_a - 2\langle x \rangle_a^2 = 2\sigma_a^2 .$$

So the relative variance is just twice the absolute variance of a single particle in this case.

c) Begorra:

$$\begin{aligned} \langle \Psi|Q|\Psi \rangle &= |c_\alpha|^2 \langle \alpha|Q|\alpha \rangle + |c_\beta|^2 \langle \beta|Q|\beta \rangle + c_\alpha^* c_\beta \langle \alpha|Q|\beta \rangle + c_\alpha c_\beta^* \langle \beta|Q|\alpha \rangle \\ &= |c_\alpha|^2 \langle \alpha|\alpha \rangle + |c_\beta|^2 \langle \beta|\beta \rangle + 2\text{Re}(c_\alpha^* c_\beta \langle \alpha|Q|\beta \rangle) , \end{aligned}$$

where we have used the definition of the Hermitian conjugate and the Hermiticity of Q : i.e., we have used

$$\langle \beta|Q|\alpha \rangle = \langle \alpha|Q^\dagger|\beta \rangle^* = \langle \alpha|Q|\beta \rangle^* .$$

Thus, we have proven the identity

$$\langle \Psi|\Psi \rangle = |c_\alpha|^2 \langle \alpha|\alpha \rangle + |c_\beta|^2 \langle \beta|\beta \rangle + 2\text{Re}(c_\alpha^* c_\beta \langle \alpha|Q|\beta \rangle) .$$

d) For identical particles and making use of the identity, we find

$$\begin{aligned} \langle x_1^2 \rangle &= \frac{1}{2(1 + \delta_{ab})} [\langle a1|x_1^2|a1\rangle\langle b2|b2\rangle + \langle a2|a2\rangle\langle b1|x_1^2|b1\rangle \pm 2\text{Re}(\langle a1|x_1^2|b1\rangle\langle b2|a2\rangle)] \\ &= \frac{1}{2(1 + \delta_{ab})} (\langle x^2 \rangle_a + \langle x^2 \rangle_b \pm 2\langle x^2 \rangle_a \delta_{ab}) \\ \langle x_2^2 \rangle &= \frac{1}{2(1 + \delta_{ab})} [\langle a1|a1\rangle\langle b2|x_2^2|b2\rangle + \langle a2|x_2^2|a2\rangle\langle b1|b1\rangle \pm 2\text{Re}(\langle a1|b1\rangle\langle b2|x_2^2|a2\rangle)] \\ &= \frac{1}{2(1 + \delta_{ab})} (\langle x^2 \rangle_a + \langle x^2 \rangle_b \pm 2\langle x^2 \rangle_a \delta_{ab}) \\ \langle x_1 x_2 \rangle &= \frac{1}{2(1 + \delta_{ab})} [\langle a1|x_1|a1\rangle\langle b2|x_2|b2\rangle + \langle a2|x_2|a2\rangle\langle b1|x_1|b1\rangle \pm 2\text{Re}(\langle a1|x_1|b1\rangle\langle b2|x_2|a2\rangle)] \\ &= \frac{1}{2(1 + \delta_{ab})} (2\langle x \rangle_a \langle x \rangle_b \pm 2|\langle x \rangle_{ab}|^2) \\ &= \frac{1}{(1 + \delta_{ab})} (\langle x \rangle_a \langle x \rangle_b \pm |\langle x \rangle_{ab}|^2) . \end{aligned}$$

Thus,

$$\langle \Delta x^2 \rangle = \frac{1}{(1 + \delta_{ab})} (\langle x^2 \rangle_a + \langle x^2 \rangle_b \pm 2\langle x^2 \rangle_a \delta_{ab} - 2\langle x \rangle_a \langle x \rangle_b \mp 2|\langle x \rangle_{ab}|^2) .$$

In the case of $|a\rangle \neq |b\rangle$, we get

$$\langle \Delta x^2 \rangle = \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2\langle x \rangle_a \langle x \rangle_b \mp 2|\langle x \rangle_{ab}|^2 .$$

Note for bosons the relative variance is smaller than for distinct particles by the term $-2|\langle x \rangle_{ab}|^2$ and for fermions it is larger by the term $2|\langle x \rangle_{ab}|^2$. Thus symmetrization clumps identical bosons more and identical fermions less than for the counterpart distinct particle case. This amounts to the exchange force.

If the $|a\rangle$ and $|b\rangle$ states don't spatially overlap, then $\langle b|x|a\rangle = 0$ and the identical-particle result is the same as distinct particle result.

In the case of $|a\rangle = |b\rangle$, we get

$$\langle \Delta x^2 \rangle = \langle x^2 \rangle_a \pm \langle x^2 \rangle_a - \langle x \rangle_a^2 \mp \langle x \rangle_a^2 .$$

For bosons, we have

$$\langle \Delta x^2 \rangle = 2\langle x^2 \rangle_a - 2\langle x \rangle_a^2 = 2\sigma_a^2$$

which is the same result as for distinct particles obtained in the part (b) answer. For fermions, we have

$$\langle \Delta x^2 \rangle = 0$$

which is what you would expect for a null state.

Redaction: Jeffery, 2001jan01

019 qfull 02400 2 5 0 moderate thinking: exchange force and infsq well

Extra keywords: (Gr-185:5.5) and the infinite square well

17. Imagine two non-interacting particles in an infinite square in the range $[0, a]$. Recall the eigen-functions for this case are

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

for $n = 1, 2, 3, \dots$. Recall also the results of the Gr-182 and Gr-29:2.5 questions.

- 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 $n = m$?
- 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 $n = m$?

SUGGESTED ANSWER:

- Using the results from the early questions we find

$$\langle \Delta x^2 \rangle = \langle x^2 \rangle_n + \langle x^2 \rangle_m - 2\langle x \rangle_n \langle x \rangle_m = a^2 \left[\frac{1}{6} - \frac{1}{2\pi^2} \left(\frac{1}{n^2} + \frac{1}{m^2} \right) \right] .$$

If $n = m$, then

$$\langle \Delta x^2 \rangle = a^2 \left(\frac{1}{6} - \frac{1}{n^2\pi^2} \right) .$$

- For this result we will have to work out a new matrix element $\langle x \rangle_{nm}$ for $n \neq m$. Behold:

$$\begin{aligned} \langle x \rangle_{nm} &= \int_0^a \psi_n^* x \psi_m dx \\ &= \frac{2}{a} \int_0^a x \sin\left(\frac{n\pi}{a}x\right) \sin\left(\frac{m\pi}{a}x\right) dx \end{aligned}$$

$$\begin{aligned}
&= \frac{2a}{\pi^2} \int_0^\pi y \sin(ny) \sin(my) dy \\
&= \frac{2a}{\pi^2} \left\{ y \left[\frac{\sin(n-m)y}{2(n-m)} - \frac{\sin(n+m)y}{2(n+m)} \right] \Big|_0^\pi - \int_0^\pi \left[\frac{\sin(n-m)y}{2(n-m)} - \frac{\sin(n+m)y}{2(n+m)} \right] dy \right\} \\
&= \frac{2a}{\pi^2} \left[\frac{\cos(n-m)y}{2(n-m)^2} - \frac{\cos(n+m)y}{2(n+m)^2} \right] \Big|_0^\pi \\
&= \frac{2a}{\pi^2} \left[-\frac{1}{(n-m)^2} + \frac{1}{(n+m)^2} \right] \left[\frac{1 - (-1)^{n-m}}{2} \right] \\
&= -\frac{8a}{\pi^2} \frac{nm}{(n^2 - m^2)^2} \left[\frac{1 - (-1)^{n-m}}{2} \right],
\end{aligned}$$

where we have used a table integral (e.g., MAT) and included the factor

$$\left[\frac{1 - (-1)^{n-m}}{2} \right]$$

which sets the matrix element to zero if $n - m$ (and thus $n + m$) is even. Using the above result and the part (a) answer we find for $n \neq m$

$$\langle \Delta x^2 \rangle = a^2 \left\{ \frac{1}{6} - \frac{1}{2\pi^2} \left(\frac{1}{n^2} + \frac{1}{m^2} \right) \pm \frac{128}{\pi^4} \frac{n^2 m^2}{(n^2 - m^2)^4} \left[\frac{1 - (-1)^{n-m}}{2} \right] \right\},$$

where the upper case is for bosons and the lower case for fermions. If $n = m$, then for bosons just

$$\langle \Delta x^2 \rangle = a^2 \left(\frac{1}{6} - \frac{1}{n^2 \pi^2} \right)$$

again. If $n = m$, then for fermions there is no allowed state or $\langle \Delta x^2 \rangle$ result.

Redaction: Jeffery, 2001jan01

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

18. There are two particles subject to separate simple harmonic oscillator (SHO) potentials. They are also coupled by a SHO interaction. The full Hamiltonian is:

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{1}{2}m_1\omega^2x_1^2 + \frac{1}{2}m_2\omega^2x_2^2 + \frac{1}{2}k(x_1 - x_2)^2,$$

where $k > 0$ which in this context means the interaction is attractive. The problem is 1-dimensional: it is in the x dimension only.

- Write down the formulae for the center-of-mass (CM) and relative (REL) coordinate and their inverses (i.e., CM coordinate X and relative x expressed in terms of x_1 and x_2).
- Transform the Hamiltonian to the center-of-mass-relative (CM-REL) coordinates (showing all the steps).
- Now show that the time-independent Schrödinger equation for the Hamiltonian separates into CM and REL time-independent Schrödinger equations. Define

$$\tilde{\omega} = \sqrt{\omega^2 + \frac{k}{\mu}} = \omega \sqrt{1 + \frac{k}{\mu\omega^2}}$$

in order to simplify the REL equation. Does the overall time-independent Schrödinger equation have an exact solution?

- Write down the general expression for the eigen-energies of the total stationary states in terms of the SHO quantum numbers n_{CM} and n_{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 $k/(\mu\omega^2) \ll 1$. Write down a first order correct expression for the energy in terms of n and n_{REL} . Give a schematic energy-level diagram.
- g) Now assume that $k/(\mu\omega^2) \gg 1$. 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_{CM} and n_{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 aren'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 eigen-spinors 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?

SUGGESTED ANSWER:

- a) For the sake of generality, let's work in three dimensions for awhile even though the problem is 1-dimensional. We can specialize when we need to to the 1-dimensional case.

Define the relative radius

$$\vec{r} = \vec{r}_2 - \vec{r}_1 ,$$

the total mass

$$M = m_1 + m_2$$

and the CM radius

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

For the inverses, we substitute for \vec{r}_2 in the formula for \vec{R} using expression $\vec{r}_2 = \vec{r} + \vec{r}_1$ which 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

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

The specializations to the 1-dimensional case are obvious.

- b) First, we need to transform kinetic energy observables. We find

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

where $i = 1$ for the upper case and $i = 2$ for the lower case. Next we find

$$\frac{\partial^2}{\partial x_i^2} = \frac{\partial^2}{\partial x^2} + \left(\frac{m_i}{M}\right)^2 \frac{\partial^2}{\partial X^2} \mp 2\frac{m_i}{M} \frac{\partial^2}{\partial x \partial X} .$$

Exactly analogous expressions hold for y and z coordinates. Thus, we find that

$$\frac{1}{m_1}\nabla_1^2 + \frac{1}{m_2}\nabla_2^2 = \frac{(m_1 + m_2)}{M^2}\nabla_{\text{CM}}^2 + \left(\frac{1}{m_1} + \frac{1}{m_2}\right)\nabla^2 = \frac{1}{M}\nabla_{\text{CM}}^2 + \frac{1}{\mu}\nabla^2 ,$$

where for simplicity here and below we only distinguish the operators with a subscripts CM and REL when needed and where we define the reduced mass by

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2} \quad \text{or} \quad \mu = \frac{m_1 m_2}{M} .$$

Second, we need to find the conversion relations needed for the potential terms. We find

$$\begin{aligned} \frac{1}{2}m_1\omega^2r_1^2 + \frac{1}{2}m_2\omega^2r_2^2 &= \frac{1}{2}\omega \left[m_1 \left(\vec{R} - \frac{m_2}{M}\vec{r} \right) \cdot \left(\vec{R} - \frac{m_2}{M}\vec{r} \right) + m_2 \left(\vec{R} + \frac{m_1}{M}\vec{r} \right) \cdot \left(\vec{R} + \frac{m_1}{M}\vec{r} \right) \right] \\ &= \frac{1}{2}\omega \left[(m_1 + m_2)R^2 + \frac{(m_1m_2^2 + m_2m_1^2)}{M^2}r^2 - 2\frac{m_1m_2}{M}\vec{R} \cdot \vec{r} + 2\frac{m_1m_2}{M}\vec{R} \cdot \vec{r} \right] \\ &= \frac{1}{2}M\omega R^2 + \frac{1}{2}\mu\omega r^2 . \end{aligned}$$

The corresponding relations for any component are analogous. Note that the nice separation into a center-of-mass SHO potential and relative SHO potential would not have been possible if the angular frequencies had been different.

In the present case, the Hamiltonian is confined to the x dimension only. We see this Hamiltonian in CM-REL coordinates must be

$$H = \frac{P^2}{2M} + \frac{p^2}{2\mu} + \frac{1}{2}M\omega^2X^2 + \frac{1}{2}\mu\omega^2x^2 + \frac{1}{2}kx^2 .$$

c) With the transformed Hamiltonian, the time-independent Schrödinger equation becomes

$$H\Psi(X, x) = H_{\text{CM}}\Psi(X, x) + H_{\text{REL}}\Psi(X, x) = E\Psi(X, x) ,$$

where we have specialized our transformations to the 1-dimensional case.

If we separate the wave function

$$\Psi(X, x) = \Psi(X)\Psi(x)$$

and divide the Schrödinger equation, we obtain

$$\frac{H_{\text{CM}}\Psi(X)}{\Psi(X)} + \frac{H_{\text{REL}}\Psi(x)}{\Psi(x)} = E .$$

Since we can vary X and x independently, it is clear that both terms on the right-hand side equal constants which we identify as E_{CM} and E_{REL} . Thus, we have separate Schrödinger equations:

$$\begin{aligned} H_{\text{CM}}\Psi(X) &= \left(\frac{P^2}{2M} + \frac{1}{2}M\omega^2X^2 \right) \Psi(X) = E_{\text{CM}}\Psi(X) \\ H_{\text{REL}}\Psi(x) &= \left(\frac{p^2}{2\mu} + \frac{1}{2}\mu\tilde{\omega}^2x^2 \right) \Psi(x) = E_{\text{REL}}\Psi(x) , \end{aligned}$$

where, as suggested, we have defined

$$\tilde{\omega} = \sqrt{\omega^2 + \frac{k}{\mu}} = \omega\sqrt{1 + \frac{k}{\mu\omega^2}} .$$

Both the CM and REL parts are SHOs, and thus have exact solutions. Ergo the total Schrödinger equation also has an exact solution.

d) The eigen-energies of the total solution are given by

$$E = E_{\text{CM}} + E_{\text{REL}} = \left(n_{\text{CM}} + \frac{1}{2} \right) \hbar\omega + \left(n_{\text{REL}} + \frac{1}{2} \right) \hbar\tilde{\omega} ,$$

where both the n_{CM} and n_{REL} quantum numbers run $0, 1, 2, 3, \dots$

e) If $k = 0$, then

$$E = (n_{\text{CM}} + n_{\text{REL}} + 1) \hbar\omega .$$

We can define a new quantum number

$$n = n_{\text{CM}} + n_{\text{REL}}$$

which labels the distinct energy levels and runs $0, 1, 2, 3, \dots$. Thus,

$$E = (n + 1)\hbar\omega .$$

The degenerate states can be labeled by

$$n_{\text{REL}}$$

which runs only $0, 1, 2, 3, \dots, n$. The degeneracy is $n + 1$. Only the ground state is not degenerate.

If one made a square array states with n_{CM} and n_{REL} labeling, respectively, infinite rows and columns, then n runs along the vertical axis labeling diagonals made of degenerate states and n_{REL} runs along the diagonal labeling the degenerate states for each n .

f) If $k/(\mu\omega^2) \ll 1$, then

$$\tilde{\omega} \approx \omega \left(1 + \frac{k}{2\mu\omega^2} \right)$$

to 1st order. We now see that

$$\begin{aligned} E &= E_{\text{CM}} + E_{\text{REL}} = \left(n_{\text{CM}} + \frac{1}{2} \right) \hbar\omega + \left(n_{\text{REL}} + \frac{1}{2} \right) \hbar\tilde{\omega} \\ &\approx \left(n_{\text{CM}} + \frac{1}{2} \right) \hbar\omega + \left(n_{\text{REL}} + \frac{1}{2} \right) \hbar\omega + \left(n_{\text{REL}} + \frac{1}{2} \right) \hbar\omega \left(\frac{k}{2\mu\omega^2} \right) \\ &= (n + 1)\hbar\omega + \left(n_{\text{REL}} + \frac{1}{2} \right) \hbar\omega \left(\frac{k}{2\mu\omega^2} \right) \end{aligned}$$

to 1st order. The k term is now a perturbation which splits the degeneracy. The n quantum number now labels a group of closely spaced levels and n_{REL} levels in a group. The energy-level diagram, I leave to your imagination.

g) If $k/(\mu\omega^2) \gg 1$, then the n quantum number is not useful. In this case one can only use the original quantum numbers n_{CM} and n_{REL} and let them run over $0, 1, 2, 3, \dots$. However, since n_{REL} accounts for large energy steps it makes sense to define orders of energy levels by their n_{REL} quantum number. Thus given n_{REL} , the zeroth level of the n_{REL} order has $n_{\text{CM}} = 0$, the 1st level has $n_{\text{CM}} = 1$, the 2nd $n_{\text{CM}} = 2$, and so on. Each order n_{REL} will be overlapped by the high levels of all lower orders. In general the levels of different orders will not be coincident however: they will be scattered about higgedly-piggedly.

If we do, however, equate to energy levels from different orders

$$\left(n_{\text{CM}} + \frac{1}{2} \right) \hbar\omega + \left(n_{\text{REL}} + \frac{1}{2} \right) \hbar\tilde{\omega} = \left(n'_{\text{CM}} + \frac{1}{2} \right) \hbar\omega + \left(n'_{\text{REL}} + \frac{1}{2} \right) \hbar\tilde{\omega}$$

and rearrange to get

$$n'_{\text{CM}} - n_{\text{CM}} = (n_{\text{REL}} - n'_{\text{REL}}) \frac{\tilde{\omega}}{\omega} ,$$

then we only get an acceptable integral solution for $n'_{\text{CM}} - n_{\text{CM}}$ for any $n_{\text{REL}} - n'_{\text{REL}}$ if $\tilde{\omega}/\omega$ is an integer. For definiteness, let's say that the primes indicate the lower order. Thus $n_{\text{REL}} - n'_{\text{REL}} \geq 0$ and $n'_{\text{CM}} - n_{\text{CM}} \geq 0$. This means that any solution of order n_{REL} is degenerate with an energy solution of each of lower orders n'_{REL} . Thus the degeneracy of any energy level is $n_{\text{REL}} + 1$ counting orders 0 through n_{REL} itself.

h) The symmetry requirement for spin-0 boson states is that on the interchange of any pair of particle coordinates, the state function stay the same. In this case the state function in terms of the individual coordinates is

$$\Psi_{n_{\text{CM}}} \left(\frac{m_1 x_1 + m_2 x_2}{M} \right) \Psi_{n_{\text{REL}}} (x_2 - x_1) ,$$

where each component state function is a one-dimensional SHO wave function. The CM component is, in fact, already symmetric on pair interchange, and so imposes no new restrictions. Since SHO wave functions are even for even quantum number and odd for odd, the REL component is symmetric for n_{REL} even and antisymmetric for n_{REL} odd. No combination of antisymmetric functions can ever be symmetric, so we must exclude all odd n_{REL} solutions: they aren't physically realizable for spin-0 bosons. Note the remaining solutions still constitute a complete set, but only for spin-0 bosons.

i) The standard eigen spinors for a 2 spin-1/2 fermion system are

$$\begin{aligned}\chi_{1,1} &= \alpha(1)\alpha(2) \\ \chi_{1,0} &= \frac{1}{\sqrt{2}}[\alpha(1)\beta(2) + \beta(1)\alpha(2)] \\ \chi_{1,-1} &= \beta(1)\beta(2)\end{aligned}$$

and

$$\chi_{0,0} = \frac{1}{\sqrt{2}}[\alpha(1)\beta(2) - \beta(1)\alpha(2)] ,$$

where the first three spinors constitute the symmetric triplet state and the last one the antisymmetric singlet state and where

$$\alpha = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \beta = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

(e.g., Morrison et al. 1991, p. 188). Since the overall eigenstate must be antisymmetric, the singlet state requires n_{REL} even and the triplet state requires n_{REL} odd. This is the only restriction.

Redaction: Jeffery, 2001jan01

019 qfull 02600 1 5 0 easy thinking: symmetrization, Slater determinant

Extra keywords: (Gr-187:5.7)

19. Say that you solve a Schrödinger equation for N identical particles to get the normalized wave function $\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots, \vec{r}_N)$. 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?

SUGGESTED ANSWER:

To symmetrize for bosons, one would just construct a Slater determinant with all the minus signs dropped. One could use position for the row coordinates and permute the variable indices or vice versa. For fermions (all in spin-up state) you would leave in the negative signs for the anticyclic permutations. To normalize the symmetrized wave function one would multiply by $1/\sqrt{N!}$ given the condition that the wave function were completely unsymmetrized initially and all the permutations led to orthogonal wave functions. Although typically one has that condition, it certainly isn't always true. Say one had $N = 2$ and $\psi(\vec{r}_1, \vec{r}_2)$ and the wave function was already, unbeknownst to you, symmetric/antisymmetric. In this case

$$\int \psi(\vec{r}_1, \vec{r}_2)^* \psi(\vec{r}_2, \vec{r}_1) dV \neq 0$$

and the correct normalization for a redundant symmetrization would not be $1/\sqrt{2}$, but $1/2$. One hopes in specific cases that one would know the symmetries of the Schrödinger equation. I imagine that symmetrization is easier said than done in general.

Redaction: Jeffery, 2001jan01

019 qfull 02700 1 5 0 easy thinking: doubly excite He decay

Extra keywords: (Gr188.58a)

20. 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.

SUGGESTED ANSWER:

If we make the first choice, the $n = 2$ shell is $\sim 4\text{ eV}$ below the continuum of the atom and $\sim 50\text{ eV}$ above the ground state of the He^+ ion. From energy conservation

$$E_{\text{eject}} + E_{\text{grd}} = 2E_{n=2}$$

or

$$E_{\text{eject}} = 2E_{n=2} - E_{\text{grd}} = -8 + 50 = 42\text{ eV} .$$

The second choice (i.e., pure hydrogenic levels) gives

$$E_{\text{eject}} = 2E_{n=2} - E_{\text{grd}} = 2\frac{-ZE_{\text{ryd}}}{n^2} - (-ZE_{\text{ryd}}) = -E_{\text{ryd}} + 2E_{\text{ryd}} = E_{\text{ryd}} = 13.6\text{ eV} ,$$

where $n = 2$, $Z = 2$, and Z_{ryd} is the Rydberg energy, of course.

Which choice is better? The hydrogenic choice is more definite: one isn't left in a quandary about what values to use. But it isn't more accurate a priori. The only way to know the best choice is to do the more detailed calculation which requires specifying the initial state precisely and finding out exactly what its energy is.

Redaction: Jeffery, 2001jan01

019 qfull 02900 2 5 0 moderate thinking: helium with bosons

Extra keywords: (Gr-188:5.9)

21. Describe qualitatively how the helium atom energy level diagram would plausibly change under the following conditions.
- Say the electrons were spin zero bosons.
 - Say the electrons were spin 1/2 bosons—a contradiction in postulates, but for the sake of argument have it so.
 - 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.

SUGGESTED ANSWER:

- In this case there would be no spin state to discuss. The total state would have to be the wave function and it would have to be symmetric. The energy level diagram would probably resemble the singlet state branch of the actual helium energy level diagram. Recall the singlet branch is spatially symmetric and spin antisymmetric.
- In this case one would still have the singlet and triplet branches of the actual helium atom. Other since the overall state would have to be symmetric, the singlet branch would correspond to the antisymmetric wave function case and the triplet branch to the symmetric wave function case. Since antisymmetric wave functions keep the electrons physically further apart, they give the lower energy branch. Thus in this case the singlet branch levels would tend to have lower energies than their triplet branch counterparts—this is the opposite of actual helium atom of course. Note the ground state single-particle wave function is non-degenerate. Thus the ground state must be a triplet spin state in when the electrons are spin 1/2 bosons so that overall state is symmetric. In the actual helium atom the ground spin state is a singlet to make the overall ground state antisymmetric.

- c) If the electrons are distinguishable, then there is no requirement for the states to have definite symmetry. The ground spatial state must be symmetric since the single-particle ground wave functions out of which it is approximately constructed are non-degenerate. However, both singlet and triplet spin states are allowed, and so the overall symmetry of the ground state could be either. Some of excited states may be spatially symmetric and antisymmetric states both with spin singlet and triplet forms. But there can be other states without definite spatial symmetry. Off hand I don't know if the overall spin state can be sans definite symmetry: i.e., the electron spins not taking a "parallel" or "antiparallel" relation. In any case the energy level diagram would be quite different I think than that of the actual helium atom. Oddly enough something somewhat like this system could be built from a helium nucleus with an electron and muon. The muon is 207.77 times the mass of the electron, and so would tend to be much deeper in the potential well of the nucleus: radius going as $1/m$ (see, e.g., Gr-137). I don't know if muonic helium has ever been studied: probably yes.

Redaction: Jeffery, 2001jan01

019 qfull 03000 2 5 0 moderate thinking: Bose-Einstein counting

Extra keywords: See Po-13 and Po-47

22. 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 $ijk\dots\ell$ is $p_i p_j p_k \dots p_\ell$ 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 insertion 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?

SUGGESTED ANSWER:

- a) As a mental procedure for finding all the possible global states, we can imagine slotting the particles into single-particle states one at a time. All possible global states can be constructed this way: could you imagine one that couldn't? Consider inserting in the first particle. There are g single-particle states, and so one can form g global particle states by inserting the first particle. Then assume that for $n - 1$ particles added, one can construct g^{n-1} distinct global states. Now to each of these global states you can add the n th particle in g ways; thus for each there are g n -particle global states. These new global states are all distinct, because the n th particle is distinct from all the particles added before. Thus for n particles there are $g^{n-1} \times g = g^n$ distinct global states. The probability of each state is just $1/g^n$ assuming the states have equal probability.
- b) Well there $n!$ ways of arranging the n insertions of sequence, but distinct sequences aren't formed by rearrangements among particles going into the same single-particle states. Let N be the number of distinct sequences. For sequences resulting in global states with the occupation number set $\{n_i\}$, we must have

$$n! = N \prod_{i=1}^g n_i! ,$$

and thus

$$N = \frac{n!}{\prod_{i=1}^g n_i!} .$$

If all the p_i are equal, then $p_i = 1/g$ and the probability of any insertion sequence is $1/g^n$ since there are n p_i factors in the probability of a sequence. The probability of any global state of occupation number set $\{n_i\}$ formed by random insertion must be

$$p(\{n_i\}) = \frac{n!}{\prod_{i=1}^g n_i} \frac{1}{g^n} .$$

The sum of the probabilities of all insertion sequences must 1. When you insert n particles in a sequence you always get a global state at the end. Thus probability for getting any global state is 1. Thus the sum of probabilities for all sequences must be 1.

Now for a more explicit proof using induction. The first step is to prove that sum of all probabilities for sequences of $n = 1$ is 1. Well we are given that $\sum_{i=1}^g p_i = 1$ and clearly the p_i are the probabilities of the sequences of $n = 1$. Thus, we have proven

$$1 = \left(\sum_{i=1}^g p_i \right)^1 .$$

The second step is to assume that all $n - 1$ sequence probabilities occur in the expansion of

$$1 = \left(\sum_{i=1}^g p_i \right)^{n-1} .$$

The third step is to insert the n th particle to any of the global states formed by a sequence of $n - 1$ particle insertations. For each sequence of $n - 1$, there are n possible sequences of n . The probability of sequences of n where the final insertion is into state i is just the probability of the sequence of $n - 1$ times p_i . It follows that

$$\left(\sum_{i=1}^g p_i \right)^{n-1} \left(\sum_{i=1}^g p_i \right) = \left(\sum_{i=1}^g p_i \right)^n$$

is the sum of the probabilities of all sequences of n . Since $\sum_{i=1}^g p_i = 1$, we find

$$1 = \left(\sum_{i=1}^g p_i \right)^n .$$

Thus the sum of all sequence of n probabilities is 1.

- c) Well there are g choices for the first state. Then there are $g-1+n$ choices for the second event which may be inserting a particle into the first state or choosing a new state. For the next there are $g-1+n-1$ choices and so on down to 1 choice. Thus we can construct $g(g-1+n)!$ factorial states according to our rule. But the order of choosing states can't matter in constructing a global state and the order of choosing particles can't matter either since they are identical. Thus the number of distinct states M must satisfy

$$g(g-1+n)! = Mg!n! ,$$

where $g!$ accounts for all possible rearrangements of the choice of states without any other changes and $n!$ for all possible rearrangements of the particle insertion order without any other changes. Therefore,

$$M = \frac{(g-1+n)!}{(g-1)!n!} .$$

The above counting procedure is isomorphic to the distinct orderings of $(g-1)$ identical partitions and n identical particles on a line. I still don't know what is the best word argument to motivate the simple mathematical steps.

- d) The probability of each distinct global state of bosons is

$$p = \frac{1}{M} = \frac{(g-1)!n!}{(g-1+n)!}$$

since all distinct global states have equal probability. Now if all particles are in one single-particle state the boson probability for the global state is just as above, but the classical probability is

$$p_{\text{cl}} = \frac{1}{g^n}$$

from the part (b) answer. To see which probability is larger consider that

$$p = \frac{1}{M} = \frac{(g-1)!n!}{(g-1+n)!} = \frac{n!}{(g-1+n)(g-2+n)\dots g} = \frac{n(n-1)\dots 1}{(g-1+n)[g-1+(n-1)]\dots (g-1+1)} .$$

Now clearly if $i/(g-1+i) \geq 1/g$ where $i \in [1, n]$, then $p \geq p_{\text{cl}}$. Let's assume that $i/(g-1+i) \geq 1/g$ and show under what condition that that leads to no contradiction. Consider the sequence of statements where the preceding implies the following:

$$\begin{aligned} \frac{i}{g-1+i} &\geq \frac{1}{g} , \\ i &\geq \frac{i-1}{g} + 1 , \\ i-1 &\geq \frac{i-1}{g} . \end{aligned}$$

The last statement is always true for allowed i and g : i.e., both integers greater than zero. The equality holds only for $g=1$ and/or $i=1$. Thus $p \geq p_{\text{cl}}$ in allowed cases. The equality only holds for $g=1$ (i.e., there is only one single-particle state and it has probability $p_1=1$ and only one global state and it has probability 1 too) and/or $n=1$ (i.e., there is only one particle).

The fact that $p \geq p_{\text{cl}}$ for the case of all the particles in one single-particle state suggests that in general the boson probabilities favor clumping particles into single-particle states more

strongly than classical probabilities. This suggestion is, in fact, true although I don't know a general way to prove it. I suppose one could define $f = \ln(p/p_{cl})$ and approximate f using Stirling's approximation (Ar-464) and then try to show that its minimum subject to the constraint of $\sum_{i=1}^g n_i = n$ is greater than 1. One could use Lagrange undetermined multipliers to impose the constraint (Ar-790). Just musing here: I don't know if this would work.

- e) Of course, any one run of 36 will only give one sample of the infinite distribution of runs of 36. But 36 is long enough that the unless one is unlucky it will approximate the mean run of 36 which is what infinite runs will give you.

When I did the experiment I got 18 head-tails, 11 heads, and 7 tails. This sample is closest to classical distribution of 1/2 for the head-tail state, 1/4 for all heads, and 1/4 for all tails:

$$p(\text{head-tail}) = \frac{2!}{11!} \frac{1}{2^2} = \frac{1}{2}, \quad p(\text{heads}) = \frac{2!}{2!0!} \frac{1}{2^2} = \frac{1}{4}, \quad \text{and} \quad p(\text{tails}) = \frac{2!}{2!0!} \frac{1}{2^2} = \frac{1}{4}.$$

The boson distribution is of course probability $(2-1)!/(2-1+2)! = 1/3$ for each distinct state. I certainly expect the classical distribution to hold since macroscopically each coin toss is independent of the other. There is no funny symmetrization requirement on macroscopic states.

Redaction: Jeffery, 2001jan01

020 qmult 00100 1 1 1 easy memory: atom defined

23. 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.

SUGGESTED ANSWER: (a)

Wrong Answers:

- b) This is a diatomic molecule.

Redaction: Jeffery, 2001jan01

020 qmult 01000 1 4 1 easy deducto-memory: central potential

24. "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

SUGGESTED ANSWER: (a)

Wrong answers:

- d) Doesn't seem to likely to work.
e) Off hand I can't think of a poorer approximation.

Redaction: Jeffery, 2001jan01

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

25. Write down the ground state electronic configurations of the atoms from hydrogen to calcium.

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

Appendix 2 Quantum Mechanics Equation Sheet

Note: This equation sheet is intended for students writing tests or reviewing material. Therefore it is 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	$a_{\text{Bohr}} = \frac{\lambda_{\text{Compton}}}{2\pi\alpha}$	$= 0.529 \text{ \AA}$
Boltzmann's constant	k	$= 0.8617 \times 10^{-6} \text{ eV K}^{-1}$ $= 1.381 \times 10^{-16} \text{ erg K}^{-1}$
Compton wavelength	$\lambda_{\text{Compton}} = \frac{h}{m_e c}$	$= 0.0246 \text{ \AA}$
Electron rest energy	$m_e c^2$	$= 5.11 \times 10^5 \text{ eV}$
Elementary charge squared	e^2	$= 14.40 \text{ eV \AA}$
Fine Structure constant	$\alpha = \frac{e^2}{\hbar c}$	$= 1/137.036$
Kinetic energy coefficient	$\frac{\hbar^2}{2m_e}$	$= 3.81 \text{ eV \AA}^2$
	$\frac{\hbar^2}{m_e}$	$= 7.62 \text{ eV \AA}^2$
Planck's constant	h	$= 4.15 \times 10^{-15} \text{ eV}$
Planck's h-bar	\hbar	$= 6.58 \times 10^{-16} \text{ eV}$
Rydberg Energy	hc	$= 12398.42 \text{ eV \AA}$
	$\hbar c$	$= 1973.27 \text{ eV \AA}$
	$E_{\text{Ryd}} = \frac{1}{2} m_e c^2 \alpha^2$	$= 13.606 \text{ eV}$

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

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

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

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

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

4 Some Operators

$$p = \frac{\hbar}{i} \frac{\partial}{\partial x} \quad p^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}$$

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

$$p = \frac{\hbar}{i} \nabla \quad p^2 = -\hbar^2 \nabla^2$$

$$H = \frac{p^2}{2m} + V(\vec{r}) = -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r})$$

$$\nabla = \hat{x} \frac{\partial}{\partial x} + \hat{y} \frac{\partial}{\partial y} + \hat{z} \frac{\partial}{\partial z} = \hat{r} \frac{\partial}{\partial r} + \hat{\theta} \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{\phi} \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi}$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}$$

5 Kronecker Delta and Levi-Civita Symbol

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

$$\varepsilon_{ijk} \varepsilon_{ilm} = \delta_{jl} \delta_{km} - \delta_{jm} \delta_{kl} \quad (\text{Einstein summation on } i)$$

6 Time Evolution Formulae

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

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

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

7 Simple Harmonic Oscillator (SHO) Formulae

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

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

$$\begin{aligned}
H_0(\beta x) = H_0(\xi) = 1 & & H_1(\beta x) = H_1(\xi) = 2\xi \\
H_2(\beta x) = H_2(\xi) = 4\xi^2 - 2 & & H_3(\beta x) = H_3(\xi) = 8\xi^3 - 12\xi
\end{aligned}$$

8 Position, Momentum, and Wavenumber Representations

$$p = \hbar k \quad E_{\text{kinetic}} = E_T = \frac{\hbar^2 k^2}{2m}$$

$$|\Psi(p, t)|^2 dp = |\Psi(k, t)|^2 dk \quad \Psi(p, t) = \frac{\Psi(k, t)}{\sqrt{\hbar}}$$

$$x_{\text{op}} = x \quad p_{\text{op}} = \frac{\hbar}{i} \frac{\partial}{\partial x} \quad Q \left(x, \frac{\hbar}{i} \frac{\partial}{\partial x}, t \right) \quad \text{position representation}$$

$$x_{\text{op}} = -\frac{\hbar}{i} \frac{\partial}{\partial p} \quad p_{\text{op}} = p \quad Q \left(-\frac{\hbar}{i} \frac{\partial}{\partial p}, p, t \right) \quad \text{momentum representation}$$

$$\delta(x) = \int_{-\infty}^{\infty} \frac{e^{ipx/\hbar}}{2\pi\hbar} dp \quad \delta(x) = \int_{-\infty}^{\infty} \frac{e^{ikx}}{2\pi} dk$$

$$\Psi(x, t) = \int_{-\infty}^{\infty} \Psi(p, t) \frac{e^{ipx/\hbar}}{(2\pi\hbar)^{1/2}} dp \quad \Psi(x, t) = \int_{-\infty}^{\infty} \Psi(k, t) \frac{e^{ikx}}{(2\pi)^{1/2}} dk$$

$$\Psi(p, t) = \int_{-\infty}^{\infty} \Psi(x, t) \frac{e^{-ipx/\hbar}}{(2\pi\hbar)^{1/2}} dx \quad \Psi(k, t) = \int_{-\infty}^{\infty} \Psi(x, t) \frac{e^{-ikx}}{(2\pi)^{1/2}} dx$$

$$\Psi(\vec{r}, t) = \int_{\text{all space}} \Psi(\vec{p}, t) \frac{e^{i\vec{p}\cdot\vec{r}/\hbar}}{(2\pi\hbar)^{3/2}} d^3p \quad \Psi(\vec{r}, t) = \int_{\text{all space}} \Psi(\vec{k}, t) \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}} d^3k$$

$$\Psi(\vec{p}, t) = \int_{\text{all space}} \Psi(\vec{r}, t) \frac{e^{-i\vec{p}\cdot\vec{r}/\hbar}}{(2\pi\hbar)^{3/2}} d^3r \quad \Psi(\vec{k}, t) = \int_{\text{all space}} \Psi(\vec{r}, t) \frac{e^{-i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}} d^3r$$

9 Commutator Formulae

$$[A, BC] = [A, B]C + B[A, C] \quad \left[\sum_i a_i A_i, \sum_j b_j B_j \right] = \sum_{i,j} a_i b_j [A_i, B_j]$$

$$\text{if } [B, [A, B]] = 0 \quad \text{then } [A, F(B)] = [A, B]F'(B)$$

$$[x, p] = i\hbar \quad [x, f(p)] = i\hbar f'(p) \quad [p, g(x)] = -i\hbar g'(x)$$

$$[a, a^\dagger] = 1 \quad [N, a] = -a \quad [N, a^\dagger] = a^\dagger$$

10 Uncertainty Relations and Inequalities

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

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

11 Probability Amplitudes and Probabilities

$$\Psi(x, t) = \langle x | \Psi(t) \rangle \quad P(dx) = |\Psi(x, t)|^2 dx \quad c_i(t) = \langle \phi_i | \Psi(t) \rangle \quad P(i) = |c_i(t)|^2$$

12 Spherical Harmonics

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}} \quad Y_{1,0} = \left(\frac{3}{4\pi}\right)^{1/2} \cos(\theta) \quad Y_{1,\pm 1} = \mp \left(\frac{3}{8\pi}\right)^{1/2} \sin(\theta) e^{\pm i\phi}$$

$$L^2 Y_{\ell m} = \ell(\ell+1) \hbar^2 Y_{\ell m} \quad L_z Y_{\ell m} = m \hbar Y_{\ell m} \quad |m| \leq \ell \quad m = -\ell, -\ell+1, \dots, \ell-1, \ell$$

0	1	2	3	4	5	6	...
<i>s</i>	<i>p</i>	<i>d</i>	<i>f</i>	<i>g</i>	<i>h</i>	<i>i</i>	...

13 Hydrogenic Atom

$$\psi_{n\ell m} = R_{n\ell}(r) Y_{\ell m}(\theta, \phi) \quad \ell \leq n-1 \quad \ell = 0, 1, 2, \dots, n-1$$

$$a_z = \frac{a}{Z} \left(\frac{m_e}{m_{\text{reduced}}} \right) \quad a_0 = \frac{\hbar}{m_e c \alpha} = \frac{\lambda_C}{2\pi \alpha} \quad \alpha = \frac{e^2}{\hbar c}$$

$$R_{10} = 2a_Z^{-3/2} e^{-r/a_Z} \quad R_{20} = \frac{1}{\sqrt{2}} a_Z^{-3/2} \left(1 - \frac{1}{2} \frac{r}{a_Z} \right) e^{-r/(2a_Z)}$$

$$R_{21} = \frac{1}{\sqrt{24}} a_Z^{-3/2} \frac{r}{a_Z} e^{-r/(2a_Z)}$$

$$R_{n\ell} = - \left\{ \left(\frac{2}{na_Z} \right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3} \right\}^{1/2} e^{-\rho/2} \rho^\ell L_{n+\ell}^{2\ell+1}(\rho) \quad \rho = \frac{2r}{nr_Z}$$

$$L_q(x) = e^x \left(\frac{d}{dx} \right)^q (e^{-x} x^q) \quad \text{Rodrigues's formula for the Laguerre polynomials}$$

$$L_q^j(x) = \left(\frac{d}{dx} \right)^j L_q(x) \quad \text{Associated Laguerre polynomials}$$

$$\langle r \rangle_{n\ell m} = \frac{aZ}{2} [3n^2 - \ell(\ell + 1)]$$

$$\text{Nodes} = (n - 1) - \ell \quad \text{not counting zero or infinity}$$

$$E_n = -\frac{1}{2} m_e c^2 \alpha^2 \frac{Z^2 m_{\text{reduced}}}{n^2 m_e} = -E_{\text{Ryd}} \frac{Z^2 m_{\text{reduced}}}{n^2 m_e} = -13.606 \frac{Z^2 m_{\text{reduced}}}{n^2 m_e} \text{ eV}$$

14 General Angular Momentum Formulae

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

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

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

$$J_{\{x \atop y\}} = \left\{ \begin{array}{c} \frac{1}{2} \\ \frac{1}{2i} \end{array} \right\} (J_+ \pm J_-) \quad J_{\pm}^{\dagger} J_{\pm} = J_{\mp} J_{\pm} = J^2 - J_z (J_z \pm \hbar)$$

$$[J_{fi}, J_{gj}] = \delta_{fg} i\hbar \varepsilon_{ijk} J_k \quad \vec{J} = \vec{J}_1 + \vec{J}_2 \quad J^2 = J_1^2 + J_2^2 + J_{1+} J_{2-} + J_{1-} J_{2+} + 2J_{1z} J_{2z}$$

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

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

15 Spin 1/2 Formulae

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

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

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

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

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

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

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

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

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

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

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

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

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

16 Time-Independent Approximation Methods

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

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

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

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

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

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

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

17 Time-Dependent Perturbation Theory

$$\pi = \int_{-\infty}^{\infty} \frac{\sin^2(x)}{x^2} dx$$

$$\Gamma_{0 \rightarrow n} = \frac{2\pi}{\hbar} |\langle n | H_{\text{perturbation}} | 0 \rangle|^2 \delta(E_n - E_0)$$

18 Interaction of Radiation and Matter

$$\vec{E}_{\text{op}} = -\frac{1}{c} \frac{\partial \vec{A}_{\text{op}}}{\partial t} \quad \vec{B}_{\text{op}} = \nabla \times \vec{A}_{\text{op}}$$

19 Box Quantization

$$kL = 2\pi n, \quad n = 0, \pm 1, \pm 2, \dots \quad k = \frac{2\pi n}{L} \quad \Delta k_{\text{cell}} = \frac{2\pi}{L} \quad \Delta k_{\text{cell}}^3 = \frac{(2\pi)^3}{V}$$

$$dN_{\text{states}} = g \frac{k^2 dk d\Omega}{(2\pi)^3 V}$$

20 Identical Particles

$$|a, b\rangle = \frac{1}{\sqrt{2}} (|1, a; 2, b\rangle \pm |1, b; 2, a\rangle)$$

$$\psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} (\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) \pm \psi_b(\vec{r}_1)\psi_a(\vec{r}_2))$$

21 Second Quantization

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

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

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

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

$$\begin{aligned}
|\vec{r}_1 s_1, \dots, \vec{r}_n s_n\rangle &= \frac{1}{\sqrt{n!}} \Psi_{s_n}(\vec{r}_n)^\dagger \dots \Psi_{s_1}(\vec{r}_1)^\dagger |0\rangle \\
\Psi_s(\vec{r})^\dagger |\vec{r}_1 s_1, \dots, \vec{r}_n s_n\rangle &= \sqrt{n+1} |\vec{r}_1 s_1, \dots, \vec{r}_n s_n, \vec{r} s\rangle \\
|\Phi\rangle &= \int d\vec{r}_1 \dots d\vec{r}_n \Phi(\vec{r}_1, \dots, \vec{r}_n) |\vec{r}_1 s_1, \dots, \vec{r}_n s_n\rangle \\
1_n &= \sum_{s_1 \dots s_n} \int d\vec{r}_1 \dots d\vec{r}_n |\vec{r}_1 s_1, \dots, \vec{r}_n s_n\rangle \langle \vec{r}_1 s_1, \dots, \vec{r}_n s_n| \quad 1 = |0\rangle \langle 0| + \sum_{n=1}^{\infty} 1_n \\
N &= \sum_{\vec{p}s} a_{\vec{p}s}^\dagger a_{\vec{p}s} \quad T = \sum_{\vec{p}s} \frac{p^2}{2m} a_{\vec{p}s}^\dagger a_{\vec{p}s} \\
\rho_s(\vec{r}) &= \Psi_s(\vec{r})^\dagger \Psi_s(\vec{r}) \quad N = \sum_s \int d\vec{r} \rho_s(\vec{r}) \quad T = \frac{1}{2m} \sum_s \int d\vec{r} \nabla \Psi_s(\vec{r})^\dagger \cdot \nabla \Psi_s(\vec{r}) \\
\vec{j}_s(\vec{r}) &= \frac{1}{2im} [\Psi_s(\vec{r})^\dagger \nabla \Psi_s(\vec{r}) - \Psi_s(\vec{r}) \nabla \Psi_s(\vec{r})^\dagger] \\
G_s(\vec{r} - \vec{r}') &= \frac{3n \sin(x) - x \cos(x)}{2x^3} \quad g_{ss'}(\vec{r} - \vec{r}') = 1 - \delta_{ss'} \frac{G_s(\vec{r} - \vec{r}')^2}{(n/2)^2} \\
v_{2\text{nd}} &= \frac{1}{2} \sum_{ss'} \int d\vec{r} d\vec{r}' v(\vec{r} - \vec{r}') \Psi_s(\vec{r})^\dagger \Psi_{s'}(\vec{r}')^\dagger \Psi_{s'}(\vec{r}') \Psi_s(\vec{r}) \\
v_{2\text{nd}} &= \frac{1}{2V} \sum_{pp'qq'} \sum_{ss'} v_{\vec{p}-\vec{p}', \vec{q}-\vec{q}, \vec{p}'+\vec{q}'} a_{\vec{p}s}^\dagger a_{\vec{q}s'}^\dagger a_{\vec{q}'s'} a_{\vec{p}'s} \quad v_{\vec{p}-\vec{p}'} = \int d\vec{r} e^{-i(\vec{p}-\vec{p}') \cdot \vec{r}} v(\vec{r})
\end{aligned}$$

22 Klein-Gordon Equation

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

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

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

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

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