Quantum Mechanics
Practice Final Exam   2011 May 6, Friday
NAME: SIGNATURE:

Instructions: There are 10 multiple-choice questions each worth 2 marks for a total of 20 marks altogether. Choose the **BEST** answer, completion, etc., and darken fully the appropriate circle on the table provided below. Read all responses carefully. **NOTE** long detailed preambles and responses won't depend on hidden keywords: keywords in such preambles and responses are bold-faced capitalized.

There are **THREE** full answer questions each worth 10 marks for a total of 30 marks altogether. Answer them all on the paper provided. It is important that you **SHOW** (**SHOW, SHOW, SHOW**) how you got the answer.

This is a **CLOSED-BOOK** exam. **NO** cheat sheets allowed. An equation sheet is provided. Calculators are permitted for calculations. Cell phones **MUST** be turned off. The test is out of 50 marks altogether.

This a 50-minute test. Remember your name (and write it down on the exam too).

Answer Table for the Multiple-Choice Questions

	a	b	c	d	e		a	b	c	d	e
1.	O	O	O	O	O	6.	O	O	O	O	O
2.	O	O	O	O	O	7.	O	O	O	O	O
3.	O	O	O	O	O	8.	O	O	O	O	O
4.	O	O	O	O	O	9.	O	O	O	O	O
5.	O	O	O	O	O	10.	O	O	O	O	O

011 qmult 00200 1 1 2 easy memory: separation of variables

1. A usual approach to getting the eigenfunctions of a Hamiltonian in multi-dimensions is:

   a) non-separation of variables.   b) separation of variables.
   c) separation of invariables.   d) non-separation of invariables.
   e) non-separation of variables/invariables.

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

Wrong Answers:
   e) A nonsense answer

Redaction: Jeffery, 2001jan01

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

2. The eigensolutions of the angular part of the Hamiltonian for the central force problem are the:

   a) linear harmonics.   b) spherical harmonics.   c) square harmonics.
   d) Pythagorean harmonics.   e) Galilean harmonics.

SUGGESTED ANSWER: (b)

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

Redaction: Jeffery, 2001jan01

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011 qmult 00510 1 4 3 easy deducto-memory: s electrons

3. "Let's play *Jeopardy*! For $100, the answer is: What the $\ell = 0$ electrons (or zero orbital angular momentum electrons) are called in spectroscopic notation."

   What are _____, Alex?

   a) the Hermitian conjugates   b) Herman's Hermits   c) s electrons
   d) p electrons   e) h electrons

SUGGESTED ANSWER: (c)

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

Redaction: Jeffery, 2001jan01

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

4. "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

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022 qmult 00100 1 1 3 easy memory: simplest quantum mechanical solid model
5. The simplest quantum mechanical solid model is arguably:

a) the hydrogen atom.   b) the helium atom.
c) the free electron gas model.   d) the infinite periodic potential model.
e) the finite periodic potential model.

SUGGESTED ANSWER: (c)

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

Wrong answers:
a) A nonsense answer.

Redaction: Jeffery, 2008jan01

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022 qmult 00110 1 1 1 easy memory: infinite square boundary conditions
6. For the free electron gas model of a solid, one common simple choice of boundary conditions is _____ conditions.

a) infinite square well   b) finite square well   c) Gaussian well
d) hydrogen atom   e) helium atom

SUGGESTED ANSWER: (a)

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

Redaction: Jeffery, 2008jan01

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022 qmult 00130 1 4 4 easy deducto-memory: periodic boundary conditions

Extra keywords: mathematical physics

7. "Let's play *Jeopardy*! For \$100, the answer is: These quantum mechanical boundary conditions for solids, also known a Born-von-Karman boundary conditions, are not realistic in most cases. They are realistic in some cases. For example, for the dimension of a solid that forms a closed loop: e.g., a solid that has donut shape can be have an angular coordinate that must be periodic by symmetry over the range $[0°, 360°]$. But whether realistic or not, it can be shown that they lead to the same average behavior as realistic boundary conditions for macroscopically large solid samples.

Why are these boundary conditions used at all? Well for one thing they are an ideal kind of boundary conditions that are completely independent of what the surface behavior of solid is. Thus, they are neutral case. For another thing they are easy to use in developments in particular when dealing with periodic potentials in a solid."

What are _____ boundary conditions, Alex?

a) infinite square well   b) aperiodic   c) Rabi-Schwinger-Baym-Sutherland
d) periodic   e) relaxed

SUGGESTED ANSWER: (d)

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

Redaction: Jeffery, 2008jan01

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

8. The formula
$$E_n^{1st} = E_n^{(0)} + \lambda \langle \psi_n^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle$$

is a:

a) 0th order perturbed energy.   b) 1st order perturbed energy.
c) 2nd order perturbed energy.   d) 1st order perturbed state.
e) 2nd order perturbed state.

SUGGESTED ANSWER: (b)

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

Redaction: Jeffery, 2001jan01

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015 qmult 00400 1 4 4 easy deducto-memory: 1st order eigen state correction

9. The formula

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

is a:

a) 0th order perturbed energy.   b) 1st order perturbed energy.
c) 2nd order perturbed energy.   d) 1st order perturbed state.
e) 2nd order perturbed state.

SUGGESTED ANSWER: (d)

Wrong Answers:

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

Redaction: Jeffery, 2001jan01

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

10. The values

$$E_{\pm} = \frac{1}{2}\left[(H_{11} + H_{22}) \pm \sqrt{(H_{11} - H_{22})^2 + 4|H_{12}|^2}\right]$$

are:

a) the stationary states of a 2×2 Hamiltonian matrix.
b) the eigen-energies of a 2×2 Hamiltonian matrix.
c) the eigen-energies of a 3×3 Hamiltonian matrix.
d) the stationary states of a 3×3 Hamiltonian matrix.
e) the 1st order non-degenerate perturbation correction energies.

SUGGESTED ANSWER: (b)

Wrong answers:

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

Redaction: Jeffery, 2008jan01

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

11. Write down the ground state electronic configurations of the neutral atoms from hydrogen (element 1) to calcium (element 20).

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

023 qfull 00140 1 3 0 easy math: the MB FD BE distributions derived

12. Consider a system consisting of quantized single-particle states and fixed total number of particles N and fixed total energy E. We make the approximation that particles can occupy only one single-particle state at time: i.e., they are not in superpositions of single-particle states. The overall microscopic state of the system is set by specifying arrangement of the particles in the single-particle states. Note that exchanging distinct particles changes the microscopic state and exchanging identical particles does not.

The set of single-particle states of the same energy E_i can be called an energy level—a term which is used in different ways in different contexts. The number of single-particle states in an energy level i is the energy level degeneracy g_i. A configuration is the set of occupation numbers $\{N_i\}$ for the energy levels of the system. The statistical weight W of a configuration is the number of distinct microscopic states that correspond to that configuration.

The fundamental axiom of statistical mechanics is that in thermodynamic equilibrium all the microscopic states are equally probable. Thermodynamic equilibrium for a system occurs when the system is not changing thermodynamically with time at the macroscopic level. In thermodynamic equilibrium, the initial conditions of the system no longer determine its macroscopic behavior and their signature in the system has been effectively erased.

The fundamental axiom implies that probability distribution for the configuration is just the normalized statistical weights and the most probable configuration is the one with the largest statistical weight. It turns out the probability distribution given by the statistical weights is extremely peaked around the most probable configuration for systems of macroscopically large numbers of particles. The macroscopic thermodynamic equilibrium state is essentially this most probable configuration. The natural logarithm the statistical weight times Boltzmann's constant k identified with the classical entropy which maximizes for thermodynamic equilibrium. Thus we have

$$S = k \ln(W) \ .$$

a) The statistical weight for the configuration for a system with distinct particles is

$$W = N! \prod_i \frac{g_i^{N_i}}{N_i!} \ .$$

Solve for the set of N_i that maximize the statistical weight subject to the constraints

$$N = \sum_i N_i \ , \qquad E = \sum_i N_i E_i \ , \qquad N_i \geq 0 \ .$$

For conventional reasons, the Lagrange multiplier for the particle number constraint should be label α and that for the energy constraint β. Use appropriate approximations to get a simple analytic formula for a maximizing N_i in which the degeneracy g_i occurs only as a leading coefficient. What is the function with the degeneracy factor suppressed and what is it called?

b) The statistical weight for the configuration for a system with identical fermions is

$$W = \prod_i \binom{g_i}{N_i} \ .$$

Repeat the requirements from part (a) for this statistical weight.

c) The statistical weight for the configuration for a system with identical bosons is

$$W = \prod_i \binom{g_i - 1 + N_i}{N_i} \ .$$

Repeat the requirements from part (a) for this statistical weight.

d) The lagrange multiplier function has an uncontrained stationary point at the maximizing values of N_i. This fact along with the 1st law of classical thermodynamics

$$dE = T\,dS - \mu\,dN$$

for the case of fixed volume but variable entropy and particle number (T being temperature and μ being the chemical potential) and the identificiation of entropy allows α and β to be determined in terms of classical thermodynamics variables. Make the determinations.

SUGGESTED ANSWER:

a) It is better and conventional to find maximizing N_i for the natural logarithm of W (i.e., for the entropy) rather than W itself. We define

$$h = \ln(W) + \alpha\left(\sum_i N_i - N\right) + \beta\left(\sum_i N_i E_i - E\right)\;,$$

where α and β are Lagrange multipliers used handle the equality constraints. The inequality constraint cannot be built into the solution procedure, but can only be used to test the consistency of the result and help eliminate unphysical results. We make the approximation that the N_i are continuous variables in making use of Lagrange multipliers.

Stationary points of h with respect to N_j in the range $[N_j, N_{j-1}]$ determined by the requirement

$$0 = h(N_j) - h(N_j - 1)\;.$$

In fact, we find only one finite, non-zero N_j value satisfying this requirement, and so all stationary points lie in the range. Since the N_i are actually integers there can be only one real stationary point in the range $[N_j, N_{j-1}]$, and there is no reason to believe the continuum approximation generates others. Even if there are multiple stationary points in the continuum approximation, they are all the same value to within our error. Our best estimate of the maximizing value in the continuum approximation is

$$N_j - \frac{1}{2}\;.$$

However the actual maximizing value must be an integer, and we judge our best estimate to be

$$\text{int}(N_j)\;,$$

where int is the function that truncates a real number to the next lowest integer or the real number itself if it is an integer. Our N_j

value turns out to be positive, and so the int function builds in the constraint that $N_i \geq 0$.

We prefer the just outlined procedure for finding the stationary point to using Stirling's approximation for the factorial functions since that approximation fails for factorial function arguments less than about 2. It's also simpler I think.

Now

$$0 = h(N_j) - h(N_j - 1) = 0 + \ln(g_j) - \ln(N_j) + \alpha + \beta E_j$$
$$N_j = g_j e^{\alpha + \beta E_j}$$
$$N_{j,\text{stationary}} = \text{int}(g_j e^{\alpha + \beta E_j}) \ .$$

The formula for maximizing occupation numbers just displayed is useful in showing the good approximation when $g_j e^{\alpha + \beta E_j}$ is a small number of order a few or less. But the int function is analytically intractable and the improvement it gives is not needed for large $g_j e^{\alpha + \beta E_j}$ values which turn out to be the overwhelmingly important cases in most cases. Thus, the most useful formula for the maximizing occupation numbers is

$$N_i = g_i e^{\alpha + \beta E} \ ,$$

where for simplicity we use the index i and make no explicit indication that the N_i are the maximizing values: context tells us when they are maximizing.

If one suppresses the degeneracy factors which are system dependent and the index i which can implicit for discrete states and is unneeded in the continuous states approximation, one obtains

$$f = e^{\alpha + \beta E_i}$$

which is called the Maxwell-Boltzmann distribution.

b) We do everything that we did in the part (a) answer, *mutatis mutandis.* Now

$$0 = h(N_j) - h(N_j - 1) = 0 - \{\ln[(g_j - N_j)!] - \ln[(g_j - (N_j - 1))!]\}$$
$$- \{\ln(N_j!) - \ln[(N_j - 1)!]\} + \alpha + \beta E_j$$
$$0 = \ln(g_j - N_j + 1) - \ln(N_j) + \alpha + \beta E_j$$
$$\ln\left(\frac{N_j}{g_j - N_j + 1}\right) = \alpha + \beta E_j$$
$$\frac{N_j}{g_j - N_j + 1} = e^{\alpha + \beta E_j}$$
$$N_j = \frac{g_j + 1}{e^{-(\alpha + \beta E_j)} + 1}$$
$$N_{j,\text{stationary}} = \text{int}\left(\frac{g_j + 1}{e^{-(\alpha + \beta E_j)} + 1}\right) \ .$$

The formula for maximizing occupation numbers just displayed is useful in showing the good approximation when $g_j/[e^{-(\alpha+\beta E_j)}+1]$ is a small number of order a few or less. But the int function is analytically intractable and the improvement it gives is not needed for large $g_j/[e^{-(\alpha+\beta E_j)}+1]$ values which turn out to be the overwhelmingly important cases in most cases. Thus, the most useful formula for the maximizing occupation numbers is

$$N_i = \frac{g_i}{e^{-(\alpha+\beta E_i)}+1} \, ,$$

where for simplicity we use the index i and make no explicit indication that the N_i are the maximizing values: context tells us when they are maximizing.

If one suppresses the degeneracy factors which are system dependent and the index i which can implicit for discrete states and is unneeded in the continuous states approximation, one obtains

$$f = \frac{g_i}{e^{-(\alpha+\beta E)}+1}$$

which is called the Fermi-Dirac distribution. We note that in the limit that $e^{-(\alpha+\beta E_i)} >> 1$ the Fermi-Dirac distribution approaches the Maxwell-Boltzmann distribution.

c) We do everything that we did in the part (a) answer, *mutatis mutandis*. Now

$$0 = h(N_j) - h(N_j-1) = \{\ln[(g_j-1+N_j)!] - \ln[(g_j-1+(N_j-1))!]\}$$
$$- \{\ln(N_j!) - \ln[(N_j-1)!]\} + \alpha + \beta E_j$$
$$0 = \ln(g_j-1+N_j) - \ln(N_j) + \alpha + \beta E_j$$

$$\ln\left(\frac{N_j}{g_j-1+N_j}\right) = \alpha + \beta E_j$$

$$\frac{N_j}{g_j-1+N_j} = e^{\alpha+\beta E_j}$$

$$N_j = \frac{g_j-1}{e^{-(\alpha+\beta E_j)}-1}$$

$$N_{j,\text{stationary}} = \text{int}\left(\frac{g_j-1}{e^{-(\alpha+\beta E_j)}-1}\right) \, .$$

The formula for maximizing occupation numbers just displayed is useful in showing the good approximation when $g_j/[e^{-(\alpha+\beta E_j)}-1]$ is a small number of order a few or less. But the int function is analytically intractable and the improvement it gives is not needed for large $g_j/[e^{-(\alpha+\beta E_j)}-1]$ values which turn out to be the overwhelmingly important cases in most cases. Thus, the most useful formula for the maximizing occupation numbers is

$$N_i = \frac{g_i}{e^{-(\alpha+\beta E_i)}-1} \, ,$$

where for simplicity we use the index i and make no explicit indication that the N_i are the maximizing values: context tells us when they are maximizing.

If one suppresses the degeneracy factors which are system dependent and the index i which can implicit for discrete states and is unneeded in the continuous states approximation, one obtains

$$f = \frac{g_i}{e^{-(\alpha+\beta E)} - 1}$$

which is called the Bose-Einstein distribution. We note that in the limit that $e^{-(\alpha+\beta E_i)} \gg 1$ the Bose-Einstein distribution approaches the Maxwell-Boltzmann distribution.

d) On general path in the space of the occupation numbers $N(t)$ (where t is a path parameter) through the constrained stationary point for $\ln(W)$, the h function has an uncontrained statationary point. Therefore,

$$0 = \frac{dh}{dt} = \frac{d\ln(W)}{dt} + \alpha\frac{dN}{dt} + \beta\frac{dE}{dt} \ ,$$

where for notational convenience N and E are now the unconstrained values of the total particle number and energy. The constrained total particle number N_{con} and E_{con} are constants and vanish in the differentiation with respect to t. By a usual convention of thermodynamics, we suppress the dt and write the last expression as a differential expression with it being implicit that the differentials stand for derivatives with respect to the path parameter of the general path. Thus, we have

$$0 = d\ln(W) + \alpha\,dN + \beta\,dE \ .$$

Using the entropy identification, this last expression becomes

$$0 = dS + k\alpha\,dN + k\beta\,dE$$

which rearranges to

$$dE = -\frac{1}{k\beta}\,dS - \frac{\alpha}{\beta}\,dN \ .$$

From the classical 1st law of thermodynamics, we now see that

$$T = -\frac{1}{k\beta} \qquad \text{and} \qquad \mu = kT\alpha \ ,$$

and thus that

$$\beta = -\frac{1}{kT} \qquad \text{and} \qquad \alpha = \frac{\mu}{kT} \ .$$

Redaction: Jeffery, 2008jan01

015 qfull 01412 3 5 0 tough thinking: 2-particle Dirac delta perturbation 2
   Extra keywords: (Gr-226:6.3)

13. The single-particle stationary states and eigen-energies for a 1-dimensional infinite square well for region $[0, a]$ are, respectively,

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \qquad \text{and} \qquad E_n = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 n^2 \ .$$

a) What is the expression for elementary 2-particle stationary states for **DISTINCT** spinless particles of the same mass? Label the particles 1 and 2 for convenience. Label the states n and n' for convenience too. What is the general expression for the energy of such 2-particle states? What are all the possible reduced energies $n^2 + n'^2$ up to 100? These energies can be called energy levels: the levels may correspond to more than one state. What are are degeneracies of the energy levels? Remember the particles are **DISTINCT**. **HINT:** You are permitted to use a computer program to generate energy levels and degeneracies. But you can find them by hand too—a little tedious, but not hard if you go at it systematically.

b) Now suppose we turn on a perturbation potential for the non-identical particles of the form

$$H^{(1)} = V(x_1, x_2) = aV_0\delta(x_1 - x_2) \ .$$

What is the expression for the diagonal matrix element

$$H_{(nn')(nn')} = \langle \psi_{nn'}(x_1, x_2)|H^{(1)}|\psi_{nn'}(x_1, x_2)\rangle \ ?$$

If you expand sine functions in exponentials evaluating, the matrix element is pretty easy, but you do have to treat the cases where $n \neq n'$ and $n = n'$ a bit differently.
   Can you do perturbation theory on all the 2-particle states?

c) What is the expression for elementary 2-particle stationary states if we replace the distinct particles by identical spinless bosons? What is the general expression for the energy of such 2-particle states? (we have turned off the perturbation potential.) What are all the possible reduced energies $n^2 + n'^2$ up to 100? These energies can be called energy levels: the levels may correspond to more than one state. What are are degeneracies of the energy levels? **HINT:** You don't have to do part (a) all over again, just *mutatis mutandis* it.)

d) Now suppose we turn on a perturbation potential of part (b) for the identical bosons. What is the expression for the diagonal matrix element

$$H_{(nn')(nn')} = \langle \psi_{nn'}(x_1, x_2)|H^{(1)}|\psi_{nn'}(x_1, x_2)\rangle \ ?$$

If you expand sine functions exponentials evaluating, the matrix element is pretty easy, but you do have to treat the cases where $n \neq n'$ and $n = n'$

a bit differently. Note the perturbation correction is a bit different from the distinct particle case. Why?

Can you do perturbation theory on all the 2-particle states?

e) What is the expression for elementary 2-particle stationary states if the 2 particles identical fermions with the same spin coordinate. Since the spin coordinates are identical, the spin part of the single-particle states are symmetrical. Don't bother writing down spinors or such. What is the general expression for the energy of such 2-particle states? What are all the possible reduced energies $n^2 + n'^2$ up to 100? **HINT:** You don't have to do part (a) all over again, just *mutatis mutandis* it.)

f) Now suppose we turn on a perturbation potential of part (b) for the identical fermions. What is the expression for the diagonal matrix element

$$H_{(nn')(nn')} = \langle \psi_{nn'}(x_a, x_b)|H^{(1)}|\psi_{nn'}(x_a, x_b)\rangle .$$

Don't whine: this is easy if you see the trick. Why do you get the simple result you get?

Can you do perturbation theory on all the 2-particle states?

g) What does the Dirac delta potential

$$V(x_a - x_b) = aV_0(x_a - x_b)$$

imply or do physically?

SUGGESTED ANSWER:

a) Behold:

$$\psi(x_a, x_b) = \psi_n(x_a)\psi_{n'}(x_b) \quad \text{and} \quad E_{n,n'} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 (n^2 + n'^2) .$$

I've put the table of reduced energy levels and degeneracies below all the parts of the question. Levels with different n and n' are double degenerate since two states correspond to these levels. But levels with $n = n'$ have degeneracy 1: i.e., they are not degenerate. Note there are 3 accidental degeneracies where distinct pairs of n and n' result in the same energy. These accidental degeneracies coould be combined and their degeneracies added, but it's useful to see them separated as long as we recognize what they are. There are 38 distinct energy levels not combining the accidental degeneracies. If we combined the accidential degeneracies, there are 35 distinct energy levels.

b) Behold:

$$H_{(nn')(nn')} = \langle \psi_{nn'}(x_1, x_2)|H^{(1)}|\psi_{nn'}(x_1, x_2)\rangle$$
$$= \int_0^a \int_0^a \psi_{nn'}(x_1, x_2)^* aV_0\delta(x_1 - x_2)\psi_{nn'}(x_1, x_2) \, dx_1 \, dx_2$$

$$= aV_0 \int_0^a \psi_{nn'}(x,x)^* \psi_{nn'}(x,x)\, dx$$

$$= aV_0 \left(\frac{2}{a}\right)^2 \int_0^a \left(\frac{e^{ikx} - e^{-ikx}}{2i}\right)^2 \left(\frac{e^{ik'x} - e^{-ik'x}}{2i}\right)^2 dx$$

$$= V_0 \frac{1}{4a} \int_0^a \left(e^{2ikx} + e^{-2ikx} - 2\right) \left(e^{2ik'x} + e^{-2ik'x} - 2\right) dx$$

$$= V_0 \frac{1}{4a} \begin{cases} 4a, & n \neq n' \\ (4+2+2)\,a, & n = n' \end{cases}$$

$$= V_0 \begin{cases} 1, & n \neq n' \\ 2, & n = n' \end{cases},$$

where we got the penultimate line by pure staring at the antepenultimate line.

We can do perturbation theory. But those states that are degenerate require a diagonalization among themselves in order to obviate infinities.

c) Behold:

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2(1 + \delta_{nn'})}} \left[\psi_n(x_1)\psi_{n'}(x_2) + \psi_n(x_2)\psi_{n'}(x_1)\right]$$

and

$$E_{n,n'} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 (n^2 + n'^2).$$

The energy levels are the same as for distinct particles. Only the degeneracies are different. All energy levels are non-degenerate, except for the 3 cases accidental degeneracy. If those levels are combined, they are all doubly degenerate. The reason for the reduction in degeneracies from the distinct particle cases is that particles 1 and 2 in single-particle states n and n' is **NOT** a different total state from particles 2 and 1 in single-particle states n and n'.

d) The diagonal matrix element is identical to that in part (b), except there is an extra factor of 2 for the case where $n \neq n'$. Thus

$$H_{(nn')(nn')} = 2V_0$$

for all a cases.

The extra factor of arises because for the Dirac delta function gives

$$\psi_{nn'}(x,x)^2 = \frac{4}{2(1 + \delta_{nn'})}\psi_n(x)^2\psi_{n'}(x)^2$$

in the integrand. That extra factor of 2 cancels out for $n = n'$, but not for $n \neq n'$. The factor of 2 is a reflection of the exchange force attraction between bosons. Symmetrization makes spinless bosons closer than they would otherwise be. Since our Dirac delta

function potential only gives a contribution for when the particles have the probability of being in the same place: clumping the particles together will increase the contribution.

We can do perturbation theory. But those states that are degenerate require a diagonalization among themselves in order to obviate infinities. But for bosons, we only have the accidental degeneracies to deal with

e) Behold:

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}} \left[\psi_n(x_1)\psi_{n'}(x_2) - \psi_n(x_2)\psi_{n'}(x_1) \right] \; ,$$

where the state with $n = n'$ is not allowed by the Pauli exclusion principle (which is a consequence of the symmetrization rule). The energies of the states are

$$E_{n,n'} = \frac{\hbar^2}{2m} \left(\frac{\pi}{a} \right)^2 (n^2 + n'^2) \; .$$

The energy levels are the same as for distinct particles, except that there are 6 levels that ruled out by the Pauli exclusion principle. All energy levels are non-degenerate, except for the 2 cases accidental degeneracy. There are only 2 accidental degeneracy cases now since one case of the accidental degeneracies for distinct particles and bosons is eliminated by the Pauli exclusion principle. If those accidental degeneracy levels are combined, they are all doubly degenerate. The main reason for the reduction in degeneracies relative to the distinct particle case is that particles 1 and 2 in single-particle states n and n' is **NOT** a different total state from particles 2 and 1 in single-particle states n and n'.

f) The diagonal matrix element is always zero for the fermions with identical spin coordinates. The zeros arise because for the Dirac delta function gives
$$\psi(x, x) = 0$$
in the integrand. The reason is that identical fermions with the same spin have zero probability of being in the same place because of the antisymmetrization of the wave function. Spatial antisymmetry makes fermions farther than they would otherwise be. Since our Dirac delta function potential only gives a contribution for when the particles have the probability of being in the same state: forbidding the particles from being the same place kills the contribution.

In fact the Dirac delta perturbation cannot affect the system at all in this case. The off-diagonal matrix elements are all zero too. Sort of makse sense: a potential that only acts when the particles have a probability of being in one place can't have an effect on a system where the particles have zero probability of being one place.

So one cannot do perturbation theory for this case, but there is no need to since effectively there is no perturbation.

g) Classically, the Dirac delta function potential only turns on when the particles are in the same place. It can be attractive (energy lowering) or repulsive (energy raising). In quantum mechanics, the Dirac delta function potential only makes a contribution for the probability density of the particles being in the same place. Now you may object that the volume of parameter space where the particles are in the same place is zero. But the Dirac delta function rises to infinity, and so even a volume zero makes a non-zero contribution. In reality there probably are no Dirac delta function potentials, but there some very sharply peaked ones. Such potentials act over a small distance and are not infinitely high: thus there is a finite volume in parameter space in which the particles can interact through the potential. They are attracted or repulsed depending on the sign of V_0.

Let's go a bit beyond the required answer.

You may ask yourself—but probably not—what is the probability that the two distinct particles are within dx of each other. Let's consider the non-identical particles for simplicity. The joint probability density for the two particles is

$$\rho(x_1, x_2)\, dx_1\, dx_2 \ .$$

We have to integrate $\rho(x_1, x_2)$ along the diagonal in in the x_1-x_2 plane. We get

$$\sqrt{2} \begin{cases} 1/a\ , & n \neq n'; \\ 2/a\ , & n = n'. \end{cases} .$$

This is result is just the part (b) answer divided by $V_0 a$ to remove the potential and multiplied by $\sqrt{2}$ which is to account for integration along the diagonal. The probability of being in a band dz in width about the diagonal neglecting the end effects and the variation in $\rho(x_a, x_b)$ perpendicular to the diagonal is

$$dP(dz) = dz\, \sqrt{2} \begin{cases} 1/a\ , & n \neq n'; \\ 2/a\ , & n = n'. \end{cases}$$

Now for a point on the edge of the band

$$dx = x_a - x_b = x\sqrt{2} + \frac{dz/2}{\sqrt{2}} - \left(x\sqrt{2} - \frac{dz/2}{\sqrt{2}} \right) = \frac{dz}{\sqrt{2}}\ ,$$

and thus $dz = \sqrt{2}\, dx$ for any point x where the perpendicular crosses the diagonal. A diagram would help. Thus the probability of find both particles with dx of each other (neglecting the end effects and the variation in $\rho(x_1, x_2)$ perpendicular to the diagonal) is

$$dP(dx) = dx\, 2 \begin{cases} 1/a\ , & n \neq n'; \\ 2/a\ , & n = n'. \end{cases}$$

Since this probability is approximate, it can't be normalized: it is valid though for $dx << a$. (I think I did this right.)

The rest of this makes me feel wuzzy right now, and so I leave correcting it *sine die*.

Now what if you add a short-range potential

$$V(y) = V_{\mathrm{c}} f(y) \ ,$$

where $y = |x_a - x_b|$, V_{c} is the potential when $y = 0$, and $f(y)$ is scaling rule for the potential that goes to zero as $y \to \infty$. Now

$$I = 2 \int_0^\infty V(y) \, dy = V_{\mathrm{c}} C \ ,$$

where the 2 accounts for the $x_a - x_b < 0$ and $x_a - x_b > 0$ cases and C a constant with units of length. Let's assume that we the y region over which $f(y)$ is significant is so small that we can always approximate the probability density as a constant there. We can then approximate

$$V(y) = V_{\mathrm{c}} f(y)$$

by

$$V(y) = V_{\mathrm{c}} C \delta(y) \ .$$

If we use this version of the Dirac delta potential instead of the previous one we get

$$H_{(nn')(nn')} = V_{\mathrm{c}} C \begin{cases} 1/a, & n \neq n'; \\ 3/(2a), & n = n'. \end{cases}$$

Thus we recoginze that $V_0 a = V_{\mathrm{c}} C$. Actually there seems no good reason to parameterized the potential in terms of a since that is a length scale of the infinite square well and not of the perturbation potential itself. Now for consistency between this paragraph and the last one, what if

$$V(y) = V_{\mathrm{c}} \begin{cases} 1, & y \leq s; \\ 0, & y > s, \end{cases}$$

where s is the width of the potential. In this case $C = 2s$, and so

$$H_{(nn')(nn')} = V_{\mathrm{c}} (2s) \begin{cases} 1/a, & n \neq n'; \\ 3/(2a), & n = n'. \end{cases}$$

The s corresponds to dx in the last paragraph expression. Thus if the particles are within $s = dx$ of each other there is an extra potential contribution with height V_{cm}. This all seems right to me: how do you all feel about it?

Table of Energy Levels

L. No.	n	n'	E_{red}	Non-Id. Deg.	Id. Bo. Deg.	Id. Fe. Deg.
1	1	1	2	1	1	0
2	1	2	5	2	1	1
3	2	2	8	1	1	0
4	1	3	10	2	1	1
5	2	3	13	2	1	1
6	1	4	17	2	1	1
7	3	3	18	1	1	0
8	2	4	20	2	1	1
9	3	4	25	2	1	1
10	1	5	26	2	1	1
11	2	5	29	2	1	1
12	4	4	32	1	1	0
13	3	5	34	2	1	1
14	1	6	37	2	1	1
15	2	6	40	2	1	1
16	4	5	41	2	1	1
17	3	6	45	2	1	1
18	1	7	50	2	1	1
19	5	5	50	1	1	0
20	4	6	52	2	1	1
21	2	7	53	2	1	1
22	3	7	58	2	1	1
23	5	6	61	2	1	1
24	1	8	65	2	1	1
25	4	7	65	2	1	1
26	2	8	68	2	1	1
27	6	6	72	1	1	0
28	3	8	73	2	1	1
29	5	7	74	2	1	1
30	4	8	80	2	1	1
31	1	9	82	2	1	1
32	2	9	85	2	1	1
33	6	7	85	2	1	1
34	5	8	89	2	1	1
35	3	9	90	2	1	1
36	4	9	97	2	1	1
37	7	7	98	1	1	0
38	6	8	100	2	1	1

Note—For non-identical particles interchanging the distinct values n and n' between the particles creates a different state. 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 and n' does not create a different state. Thus for bosons the degeneracy is always 1 for each energy level. For fermions, if $n = n'$ no state is allowed by the Pauli exclusion principle and the degeneracy is zero. There are energy levels below 100 that have one of n or n' greater than 7. I have included these for completeness. Note that there are three pairs of energy levels with each one of the pair having the same reduced energies: 50, 65, and 85. These pairs should be combined, but that is tricky to computationally and it is convenient to see them separately. These pairs are examples of accidental degeneracies: different pairs of n and n' leading to the same energy. For each accidental degeneracy we could create one combined energy level: the degeneracies of the pairs just add.

Fortran 95 Code

```
!23456789a123456789b123456789c123456789d123456789e123456789f123456789g12
!
! State determines the reduced energies and
degeneracies for
! 2 non-interacting particles in an infinite square
well.
!
```

```fortran
!
      program state
      implicit none
!
      integer, parameter :: ndble=kind(0.d0)
      integer, parameter :: nprecision=ndble
      integer, parameter :: nemax=100
!
      integer :: i,j
      integer :: ien(nemax,6)
      integer :: iorder(nemax)
      integer :: istate
      integer :: itmp
      integer :: nmax
!
      nmax=ceiling(sqrt(real(nemax,nprecision)))
!
      istate=0
      do410:  do i=1,nmax
       do420:  do j=i,nmax
        itmp=i**2+j**2
        if(itmp .gt. nemax) exit do420
        istate=istate+1
        ien(istate,1)=itmp
        ien(istate,2)=i
        ien(istate,3)=j
        ien(istate,5)=1                ! identical bosons
        if(i .ne. j) then
           ien(istate,4)=2       ! distinct
particles.
           ien(istate,6)=1       ! identical fermions
          else
           ien(istate,4)=1       ! distinct
particles.
           ien(istate,6)=0       ! identical
fermions.
         end if
       end do do420
      end do do410
!
      print*,'Before order.'
      call order(istate,ien(1,1),iorder)
      print*,'After order.'
!
      if(mod(itmp,2) .eq. 0) then
         itmp=istate/2
        else
```

```
            itmp=istate/2+1
            ien(istate+1,1:6)=0
         end if
   !
         print*
         do430: do i=1,istate

print910,i,ien(iorder(i),2),ien(iorder(i),3),ien(iorder(i),1),
&
         &
ien(iorder(i),4),ien(iorder(i),5),ien(iorder(i),6)
         end do do430
   !
         print*
         write(*,910)
&
         &
(i,ien(iorder(i),2),ien(iorder(i),3),ien(iorder(i),1),
&
         &
ien(iorder(i),4),ien(iorder(i),5),ien(iorder(i),6),
&
         &
i+itmp,ien(iorder(i+itmp),2),ien(iorder(i+itmp),3),
&
         &          ien(iorder(i+itmp),1),
&
         &
ien(iorder(i+itmp),4),ien(iorder(i+itmp),5),
&
         &          ien(iorder(i+itmp),6),
         &  i=1,itmp)
   !
     910 format((i3,13('&',i3)),'\\cr')    ! For some
reason, the
   !                                       ! brackets are
needed.
   !
         end program state
   !
   !23456789a123456789b123456789c123456789d123456789e123456789f123456789g12
   !
   ! A bubble sort.  Bubble sorts are very inefficient,
but they
   ! are easy to code and remember.
   !
         subroutine order(istate,ien,iorder)
```

```
      implicit none
      integer :: i,j
      integer :: ien(istate)
      integer :: iorder(istate)
      integer :: istate
      integer :: itmp
!
!       print*,istate
!
      do410: do i=1,istate
       iorder(i)=i
!        print*,i,ien(i)
      end do do410
!
      do420: do i=istate,2,-1
       do430: do j=2,i
        if(ien(iorder(j-1)) .gt. ien(iorder(j))) then
           itmp=iorder(j-1)
           iorder(j-1)=iorder(j)
           iorder(j)=itmp
        end if
       end do do430
      end do do420
!
!        do i=1,istate
!         write(*,*) i,ien(i),iorder(i),ien(iorder(i))
!         write(*,'(3i5)') i,ien(i),ien(iorder(i))
!        end do
!
      end subroutine order
!
!23456789a123456789b123456789c123456789d123456789e123456789f123456789g12
```

Redaction: Jeffery, 2001jan01

Appendix 2 Quantum Mechanics Equation Sheet

Note: This equation sheet is intended for students writing tests or reviewing material. Therefore it neither intended to be complete nor completely explicit. There are fewer symbols than variables, and so some symbols must be used for different things.

---

1 Constants not to High Accuracy

Constant Name	Symbol	Derived from CODATA 1998
Bohr radius	$a_{\mathrm{Bohr}} = \dfrac{\lambda_{\mathrm{Compton}}}{2\pi\alpha}$	$= 0.529\,\text{Å}$
Boltzmann's constant	k	$= 0.8617 \times 10^{-6}\,\text{eV}\,\text{K}^{-1}$
		$= 1.381 \times 10^{-16}\,\text{erg}\,\text{K}^{-1}$
Compton wavelength	$\lambda_{\mathrm{Compton}} = \dfrac{h}{m_e c}$	$= 0.0246\,\text{Å}$
Electron rest energy	$m_e c^2$	$= 5.11 \times 10^5\,\text{eV}$
Elementary charge squared	e^2	$= 14.40\,\text{eV}\,\text{Å}$
Fine Structure constant	$\alpha = \dfrac{e^2}{\hbar c}$	$= 1/137.036$
Kinetic energy coefficient	$\dfrac{\hbar^2}{2m_e}$	$= 3.81\,\text{eV}\,\text{Å}^2$
	$\dfrac{\hbar^2}{m_e}$	$= 7.62\,\text{eV}\,\text{Å}^2$
Planck's constant	h	$= 4.15 \times 10^{-15}\,\text{eV}$
Planck's h-bar	$\hbar$	$= 6.58 \times 10^{-16}\,\text{eV}$
	hc	$= 12398.42\,\text{eV}\,\text{Å}$
	$\hbar c$	$= 1973.27\,\text{eV}\,\text{Å}$
Rydberg Energy	$E_{\mathrm{Ryd}} = \dfrac{1}{2}m_e c^2 \alpha^2$	$= 13.606\,\text{eV}$

---

2 Some Useful Formulae

$$\text{Leibniz's formula} \qquad \frac{d^n(fg)}{dx^n} = \sum_{k=0}^{n} \binom{n}{k} \frac{d^k f}{dx^k} \frac{d^{n-k}g}{dx^{n-k}}$$

$$\text{Normalized Gaussian} \qquad P = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x - \langle x \rangle)^2}{2\sigma^2} \right]$$

---

3 Schrödinger's Equation

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

22

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

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

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

4 Some Operators

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

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

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

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

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

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

5 Kronecker Delta and Levi-Civita Symbol

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

$$\varepsilon_{ijk}\varepsilon_{i\ell m} = \delta_{j\ell}\delta_{km} - \delta_{jm}\delta_{k\ell} \qquad \text{(Einstein summation on } i\text{)}$$

6 Time Evolution Formulae

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

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

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

7 Simple Harmonic Oscillator (SHO) Formulae

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

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

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

8 Position, Momentum, and Wavenumber Representations

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

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

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

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

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

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

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

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

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

9 Commutator Formulae

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

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

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

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

10 Uncertainty Relations and Inequalities

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

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

11 Probability Amplitudes and Probabilities

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

12 Spherical Harmonics

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

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

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

13 Hydrogenic Atom

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

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

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

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

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

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

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

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

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

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

---

14 General Angular Momentum Formulae

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

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

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

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

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

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

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

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15 Spin 1/2 Formulae

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

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

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

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

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

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

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

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

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

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

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

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

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

16 Time-Independent Approximation Methods

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

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

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

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

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

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

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

17 Time-Dependent Perturbation Theory

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

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

18 Interaction of Radiation and Matter

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

19 Box Quantization

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

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

20 Identical Particles

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

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

21 Second Quantization

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

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

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

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

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

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

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

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

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

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

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

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

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

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

22 Klein-Gordon Equation

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

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

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

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

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