Quantum Mechanics
Qualifying Exam - August 2014

Notes and Instructions

- There are 6 problems. Attempt them all as partial credit will be given.
- Write your alias on the top of every page of your solutions
- Number each page of your solution with the problem number and page number (e.g. Problem 3, p. 2/4 is the second of four pages for the solution to problem 3.)
- You must show all your work to receive full credit.

Possibly useful formulas:

Pauli matrices

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

Laplacian in spherical coordinates

$$\nabla^2\psi = \frac{1}{r}\frac{\partial^2}{\partial r^2}r\psi + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\psi}{\partial\theta}) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\psi.$$

One dimensional simple harmonic oscillator operators:

$$X = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger), \qquad P = -i\sqrt{\frac{\hbar m\omega}{2}}(a - a^\dagger)$$

Spherical Harmonics:

$$\begin{aligned}
Y_0^0(\theta,\phi) &= \frac{1}{\sqrt{4\pi}} \\
Y_1^0(\theta,\phi) &= \sqrt{\frac{3}{4\pi}}\cos\theta \\
Y_1^{\pm1}(\theta,\phi) &= \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi} \\
Y_2^0(\theta,\phi) &= \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1) \\
Y_2^{\pm1}(\theta,\phi) &= \mp\sqrt{\frac{15}{8\pi}}(\sin\theta\cos\theta)\, e^{\pm i\phi} \\
Y_2^{\pm2}(\theta,\phi) &= \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{\pm 2i\phi}
\end{aligned}$$

PROBLEM 1: Stationary and Non-Statonary States

Consider a quantum system whose particles are in the following state:

$$\Psi(x,t) = \frac{1}{\sqrt{8}}\psi_1(x)\mathrm{e}^{-iE_1t/\hbar} - i\sqrt{\frac{3}{8}}\psi_3(x)\mathrm{e}^{-iE_3t/\hbar} + \frac{1}{\sqrt{2}}\psi_5(x)\mathrm{e}^{-iE_5t/\hbar}, \tag{1}$$

where $\psi_n(x)$, $n = 1, 2, 3\ldots$ are stationary states of the Hamiltonian governing the system,

$$H\psi_n(x) = E_n\psi(x).$$

Answer the following questions:

a) Do you expect $\langle x\rangle$, $\langle x^2\rangle$ and $\langle E\rangle$ to be time dependent or time independent? Discuss briefly, but do not calculate. (2 Points)

b) Is the uncertainty ΔE positive, negative or zero? Is ΔE time dependent or time independent? Again, discuss briefly but do not calculate. (2 Points)

c) Is $\Psi(t)$ above a solution of the time dependent Schroedinger equation? Demonstrate. (2 Points)

d) If the stationary states $\psi_1(x)$, $\psi_3(x)$ and $\psi_5(x)$ are eigenstates of the harmonic oscillator, will any of your answers to part a) change? Justify. (2 Points)

e) Now assume the particles are in the state

$$\Psi(x,t) = \psi_3(x)\mathrm{e}^{-iE_3t/\hbar}.$$

Answer parts a) and b) for this state. (2 Points)

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Quantum #1

a) Operators that commute with the Hamiltonian will be time independent. Since in general $[H, x] \neq 0$, $[H, x^2] \neq 0$, and $[H, E] = 0$, we would expect $\langle x \rangle$ and $\langle x^2 \rangle$ to vary with time while $\langle E \rangle$ will not

b) $\Delta E = \sqrt{\langle E^2 \rangle - \langle E \rangle^2}$

* From this equation, we know ΔE cannot be negative and there is no reason to expect $\langle E^2 \rangle = \langle E \rangle$, thus our answer should not be 0. ΔE should be time independent as $[E^2, E] = 0$ and thus $[H, E^2] = 0$

c) The time-dependent Schrödinger eqn is:

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = H|\psi\rangle \quad \text{where } H|\psi_n\rangle = E_n|\psi\rangle$$

$$|\psi\rangle = \frac{1}{\sqrt{8}} e^{-iE_1 t/\hbar}|\psi_1\rangle - i\sqrt{3/8}\, e^{-iE_3 t/\hbar}|\psi_3\rangle + \frac{1}{\sqrt{2}} e^{-iE_5 t/\hbar}|\psi_5\rangle$$

$$\Rightarrow H|\psi\rangle = \frac{E_1}{\sqrt{8}} e^{-iE_1 t/\hbar}|\psi_1\rangle - E_3 i\sqrt{3/8}\, e^{-iE_3 t/\hbar}|\psi_3\rangle + \frac{E_5}{\sqrt{2}} e^{-iE_5 t/\hbar}|\psi_5\rangle$$

$$i\hbar \frac{\partial}{\partial t}|\psi\rangle = i\hbar\left[\frac{-iE_1/\hbar}{\sqrt{8}} e^{-iE_1 t/\hbar}|\psi_1\rangle + \frac{i^2 E_3}{\hbar}\sqrt{3/8}\, e^{-iE_3 t/\hbar}|\psi_3\rangle + \frac{-iE_5}{\hbar}\sqrt{\frac{1}{2}}\, e^{-iE_5 t/\hbar}|\psi_5\rangle\right.$$

$$= \frac{E_1}{\sqrt{8}} e^{-iE_1 t/\hbar}|\psi_1\rangle - iE_3\sqrt{3/8}\, e^{-iE_3 t/\hbar}|\psi_3\rangle + \frac{E_5}{\sqrt{2}} e^{-iE_5 t/\hbar}|\psi_5\rangle$$

$\therefore$ $|\psi\rangle$ is a solution to time dependent Schrödinger Eqn

d) If we now specify that $|\psi_n\rangle$ are the states of the SHO, the only answer that changes from part a is $\langle x \rangle$ should now be time independent since $\langle x \rangle = 0$

e) If $|\psi\rangle = e^{-iE_3 t/\hbar}|\psi_3\rangle$, All our answers in part a will be time independent b/c $|\psi_3\rangle$ is a stationary state and the time dependences will cancel out $(e^{iE_3 t/\hbar} \cdot e^{-iE_3 t/\hbar} = 1)$ Additionally, since we now definitely know E $\langle E \rangle^2 = \langle E^2 \rangle$ which means $\Delta E = 0$

PROBLEM 2: Oscillator Model of Angular Momentum

Arbitrary angular momentum can be constructed from spin-1/2. The latter can be described in terms of the Pauli matrices

$$\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}.$$

The construction of a general angular momentum can be done by introducing two sets of independent harmonic oscillators, in terms of creation ($a_\zeta^\dagger$) and annihilation (a_ζ) operators,

$$[a_+, a_-] = 0, \quad [a_+^\dagger, a_-^\dagger] = 0, \quad [a_\zeta, a_{\zeta'}^\dagger] = \delta_{\zeta,\zeta'},$$

with $\zeta, \zeta' = \pm$ indexing oscillators of type $\pm$. Now define

$$\mathbf{J} = \frac{\hbar}{2} a^\dagger \boldsymbol{\sigma} a,$$

where a is a two component operator,

$$a = \begin{pmatrix} a_+ \\ a_- \end{pmatrix}.$$

a) Given the form of the Pauli matrices, give the explicit form for J_x, J_y, J_z in terms of $a_\zeta^\dagger$ and a_ζ operators (2 Points).

b) Show that $J_\pm = J_x \pm iJ_y$ have particularly simple forms in terms of a_ζ and $a_\zeta^\dagger$ operators (1 Point).

c) Compute the commutator $[J_x, J_y]$. How is this generalized for the other components? (2 Points)

d) Show that

$$J^2 = J_z^2 + J_+J_- + i[J_x, J_y],$$

and then write this in terms of the number operators for the two harmonic oscillators,

$$n_+ = a_+^\dagger a_+, \quad n_- = a_-^\dagger a_-.$$

Show that this implies that the eigenvalues of J^2 are $j(j+1)\hbar^2$, where j is an integer or an integer plus $\frac{1}{2}$ (Hint: apply the J^2 operator in the two harmonic oscillator state $|n_+, n_-\rangle$) (3 Points).

e) Using the properties of the harmonic oscillators, show that the state in which J^2 has the eigenvalue $j(j+1)\hbar$ and $J_z = m\hbar$ can be constructed from the state in which both n_+ and n_- have the value zero, $|0\rangle$, by

$$|jm\rangle = \frac{(a_+^\dagger)^{j+m}}{\sqrt{(j+m)!}} \frac{(a_-^\dagger)^{j-m}}{\sqrt{(j-m)!}} |0\rangle.$$

(2 Points)

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Quantum #2

a) Given $\vec{J} = \frac{\hbar}{2} a^{\dagger} \vec{\sigma} a$ where $a = \langle a_+, a_- \rangle$

$$J_x = \frac{\hbar}{2} a^{\dagger} \sigma_x a$$
$$= \frac{\hbar}{2} [a_+^{\dagger} \; a_-^{\dagger}] \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} a_+ \\ a_- \end{bmatrix}$$
$$= \frac{\hbar}{2} [a_+^{\dagger} \; a_-^{\dagger}] \begin{bmatrix} a_- \\ a_+ \end{bmatrix}$$
$$= \frac{\hbar}{2} (a_+^{\dagger} a_- + a_-^{\dagger} a_+)$$

$$J_y = \frac{\hbar}{2} a^{\dagger} \sigma_y a$$
$$= \frac{\hbar}{2} [a_+^{\dagger} \; a_-^{\dagger}] \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} a_+ \\ a_- \end{bmatrix}$$
$$= \frac{\hbar}{2} [a_+^{\dagger} \; a_-^{\dagger}] \begin{bmatrix} -i a_- \\ i a_+ \end{bmatrix}$$
$$= \frac{\hbar}{2} (-i a_+^{\dagger} a_- + i a_-^{\dagger} a_+)$$

$$J_z = \frac{\hbar}{2} [a_+^{\dagger} \; a_-^{\dagger}] \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} a_+ \\ a_- \end{bmatrix}$$
$$= \frac{\hbar}{2} [a_+^{\dagger} \; a_-^{\dagger}] \begin{bmatrix} a_+ \\ -a_- \end{bmatrix}$$
$$= \frac{\hbar}{2} [a_+^{\dagger} a_+ - a_-^{\dagger} a_-]$$

b) $J_{\pm} = J_x \pm i J_y$

$$\hookrightarrow J_+ = \frac{\hbar}{2} [a_+^{\dagger} a_- + a_-^{\dagger} a_+] + i \left(\frac{-i\hbar}{2} [a_+^{\dagger} a_- + a_-^{\dagger} a_+] \right)$$
$$= \frac{\hbar}{2} [a_+^{\dagger} a_- + a_-^{\dagger} a_+] + \frac{\hbar}{2} [a_+^{\dagger} a_- - a_-^{\dagger} a_+]$$
$$= \hbar [a_+^{\dagger} a_-]$$

$$\hookrightarrow J_- = \frac{\hbar}{2} [a_+^{\dagger} a_- + a_-^{\dagger} a_+] - i \left(\frac{-i\hbar}{2} [a_+^{\dagger} a_- - a_-^{\dagger} a_+] \right)$$
$$= \frac{\hbar}{2} [a_+^{\dagger} a_- + a_-^{\dagger} a_+] - \frac{\hbar}{2} [a_+^{\dagger} a_- - a_-^{\dagger} a_+]$$
$$= h [a_-^{\dagger} a_+]$$

c) $[J_x, J_y] = J_x J_y - J_y J_x$

$$= \frac{i\hbar^2}{4} \left([a_+^{\dagger} a_- + a_-^{\dagger} a_+][a_-^{\dagger} a_+ - a_+^{\dagger} a_-] - [a_-^{\dagger} a_+ - a_+^{\dagger} a_-][a_+^{\dagger} a_- + a_-^{\dagger} a_+] \right)$$
$$= \frac{i\hbar^2}{4} \left(a_+^{\dagger} a_- a_-^{\dagger} a_+ + \cancel{a_-^{\dagger} a_+ a_-^{\dagger} a_+} - a_+^{\dagger} \cancel{a_- a_+^{\dagger} a_-} - a_-^{\dagger} a_+ a_+^{\dagger} a_- - a_-^{\dagger} a_+ a_+^{\dagger} a_- \right.$$
$$\left. - \cancel{a_-^{\dagger} a_+ a_-^{\dagger} a_+} + a_+^{\dagger} \cancel{a_- a_+^{\dagger}} a_- + a_+^{\dagger} a_- a_-^{\dagger} a_+ \right)$$
$$= \frac{i\hbar^2}{4} \left(2 a_+^{\dagger} a_- a_-^{\dagger} a_+ - 2 a_-^{\dagger} a_+ a_+^{\dagger} a_- \right)$$

#2 (cont.)

c) $$[J_x, J_y] = \frac{i\hbar^2}{2}\left(a_+^\dagger \cancel{a_- a_-^\dagger}^{\,1} a_+ - a_-^\dagger \cancel{a_+ a_+^\dagger}^{\,1} a_-\right)$$

$$= \frac{i\hbar^2}{2}\left(a_+^\dagger a_+ - a_-^\dagger a_-\right)$$

$$= i\hbar J_z$$

$\Rightarrow$ Angular momentum operators will generalize as $[J_i, J_j] = i\hbar \epsilon_{ijk} J_k$

d) $$J^2 = J_x^2 + J_y^2 + J_z^2$$

$$= J_z^2 + (J_x^2 + J_y^2)$$

$$= J_z^2 + (J_x + iJ_y)(J_x - iJ_y) \underline{- iJ_yJ_x + iJ_xJ_y}$$

$$= J_z^2 + J_+J_- + i[J_x, J_y]$$

eliminate cross terms in expansion

* Rewriting this in terms of the oscillators

$$= \frac{\hbar^2}{4}[a_+^\dagger a_+ - a_-^\dagger a_-]^2 + \hbar^2 a_+^\dagger a_- a_-^\dagger a_+ + i(i\hbar J_z)$$

$$= \frac{\hbar^2}{4}[a_+^\dagger a_+ a_+^\dagger a_+ - a_+^\dagger a_+ a_-^\dagger a_- - a_-^\dagger a_- a_+^\dagger a_+ + a_-^\dagger a_- a_-^\dagger a_-] + \hbar^2 a_+^\dagger a_- a_-^\dagger a_+$$
$$- \frac{\hbar^2}{2}[a_+^\dagger a_+ - a_-^\dagger a_-]$$

$$= \frac{\hbar^2}{4}[a_+^\dagger a_+ - a_+^\dagger a_+ a_-^\dagger a_- - a_-^\dagger a_- a_+^\dagger a_+ + a_-^\dagger a_-] + \hbar^2 a_+^\dagger a_+ - \frac{\hbar^2}{2}[a_+^\dagger a_+ - a_-^\dagger a_-]$$

$$= \frac{\hbar^2}{4}[n_+ - n_+n_- - n_-n_+ + n_-] + \hbar^2 n_+ - \frac{\hbar^2}{2}[n_+ - n_-]$$

$$= \frac{\hbar^2}{4}[3n_+ - n_+n_- - n_-n_+ - n_-]$$

$$= \ldots \quad ??$$

PROBLEM 3: Perturbation Theory

Consider a particle of mass m trapped inside a 1D parabolic potential

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

where ω sets the frequency of oscillation inside the potential.

a) If the particle is perturbed by a *static* potential

$$V_I = \alpha x,$$

with α small, compute energy correction of the energy levels in the lowest order where the result is non-zero. (3 Points)

b) What is the pertubed ket in the ground state? Compute the expectation value $\langle x \rangle$ in this state. Interpret the sign of $\langle x \rangle$. (3 Points)

c) Assume from now on that $\alpha = 0$. Imagine that the particle is charged and sits in the ground state at $t = -\infty$. Suppose an electric field is gradually tuned on, increases to a maximum at $t = 0$ and then slowly dies away,

$$V_I'(t) = -e|\mathbf{E}|x\, \mathrm{e}^{-t^2/\tau^2},$$

where e is the electric charge, and $\mathbf{E}$ is the electric field . Write down the general expression for the amplitude of transition from a generic level i to level f. (Do not solve the integral yet) (2 Points).

d) Evaluate the probability of having the particle in the first excited state at $t = +\infty$. (2 Points).

Hint: $\int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{-t^2/\tau^2} \mathrm{e}^{i\omega t} = \sqrt{\pi}\tau\, \mathrm{e}^{-\omega^2\tau^2/4}$

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Quantum #3

a) In general, our first order energy correction is $\Delta E^{(1)} = \langle n^{(0)}|V'|n^{(0)}\rangle$

$\hookrightarrow V = \frac{1}{2}m\omega^2 x^2 \rightarrow$ SHO

$V' = \alpha x = \alpha\left(\sqrt{\frac{\hbar}{2m\omega}}\,[a^\dagger + a]\right)$

$$\Rightarrow \Delta E^{(1)} = \langle n|\alpha\sqrt{\tfrac{\hbar}{2m\omega}}(a^\dagger + a)|n\rangle$$

$$= \alpha\sqrt{\tfrac{\hbar}{2m\omega}}\ \langle n|a^\dagger + a|n\rangle$$

$$= \alpha\sqrt{\tfrac{\hbar}{2m\omega}}\left[\cancel{\langle n|a^\dagger|n\rangle}^{0} + \cancel{\langle n|a|n\rangle}^{0}\right]$$

*results will go to 0 by orthogonality $\langle n|m\rangle = \delta_{nm}$

Our second order correction is generally: $\Delta E^{(2)} = \sum\limits_{k\neq n}' \frac{|V_{kn}|^2}{E_n^{(0)} - E_k^{(0)}}$

$$\Rightarrow \Delta E^{(2)} = \sum_{k\neq n}' \frac{|\langle k|V'|n\rangle|^2}{\hbar\omega[(n+1/2)-(k+1/2)]}$$

$$= \sum_{k\neq n}' \frac{|\langle k|\alpha\sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a)|n\rangle|^2}{\hbar\omega(n-k)}$$

$$= \frac{\alpha^2\hbar}{2m\omega}\cdot\frac{1}{\hbar\omega}\sum_{k\neq n}' \frac{|\langle k|a^\dagger + a|n\rangle|^2}{(n-k)}$$

$$= \frac{\alpha^2}{2m\omega^2}\sum_{k\neq n}' \frac{|\langle k|n+1\rangle\sqrt{n+1} + \langle k|n-1\rangle\sqrt{n}|^2}{n-k}$$

$$= \frac{\alpha^2}{2m\omega^2}\sum_{k\neq n}' \frac{|\sqrt{n+1}\,\delta_{k,n+1} + \sqrt{n}\,\delta_{k,n-1}|^2}{n-k}$$

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

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

$$= \frac{-\alpha^2}{2m\omega}$$

#3 (cont.)

b) The formula for the first order correction to the wave function is:

$$|n^{(1)}\rangle = \sum_{k\neq n}' \frac{\langle k|V'|n\rangle}{E_n - E_k} |k^{(0)}\rangle$$

$$= \sum_{k\neq n}' \frac{\alpha\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\,\delta_{k,n+1} + \sqrt{n}\,\delta_{k,n-1}\right)}{\hbar\omega(n-k)} |k^{(0)}\rangle$$

$$= \left(\frac{\alpha^2}{2m\hbar\omega^3}\right)^{1/2} \left(\frac{\sqrt{n+1}}{n-(n+1)}|n+1\rangle + \frac{\sqrt{n}}{n-(n-1)}|n-1\rangle\right)$$

$$= \left(\frac{\alpha^2}{2m\hbar\omega^3}\right)^{1/2} \left(\sqrt{n+1}\,|n+1\rangle - \sqrt{n}\,|n-1\rangle\right)$$

* but since we are in the ground state $n=0$, and $|-1\rangle = 0$

$$= -\left(\frac{\alpha^2}{2m\hbar\omega^3}\right)^{1/2} |1\rangle$$

* Our full state is now $|\psi\rangle = |0\rangle - \left(\frac{\alpha^2}{2m\hbar\omega^3}\right)^{1/2}|1\rangle$

$$\Rightarrow \langle x\rangle = \langle\psi|x|\psi\rangle; \quad x = \sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a)$$

$$= \overbrace{\langle 0|x|0\rangle}^{0} - \left(\frac{\alpha^2}{2m\hbar\omega^3}\right)^{1/2}\langle 0|x|1\rangle - \left(\frac{\alpha^2}{2m\hbar\omega}\right)^{1/2}\langle 1|x|0\rangle + \frac{\alpha^2}{2m\hbar\omega^3}\overbrace{\langle 1|x|1\rangle}^{0}$$

$$= -\left(\frac{\alpha^2}{2m\hbar\omega^3}\right)^{1/2}\left[\langle 0|\sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a)|1\rangle + \langle 1|\sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a)|0\rangle\right]$$

$$= -\left(\frac{\alpha^2}{4m^2\omega^4}\right)^{1/2}\left[\overbrace{\langle 0|a^\dagger|1\rangle}^{0} + \langle 0|a|1\rangle + \langle 1|a^\dagger|0\rangle + \overbrace{\langle 1|a|0\rangle}^{0}\right]$$

$$= \frac{-\alpha}{2m\omega^2}\left[\langle 0|0\rangle + \langle 1|1\rangle\right]$$

$$= \frac{-\alpha}{m\omega^2}$$

* The expectation value being negative implies that the potential is deeper on the negative side than the unperturbed potential

#3 (cont.)

c) The transition probability is: (assumes a two state problem of i, f as states

$$c_n^{(1)} = \frac{-i}{\hbar}\int_{t_0}^{t} e^{-i\omega_{ni}t'} V_{ni}(t')\,dt', \quad \omega_{ni} = \omega_n - \omega_f, \quad E = \hbar\omega$$

$$V = -e|\vec{E}|x e^{-t^2/\tau^2}$$

*Simplifying the equation, we see:

$$V_{ni} = \langle f|V|i\rangle$$

$$= \langle f|-e|\vec{E}|x e^{-t^2/\tau^2}|i\rangle$$

$$= -e|\vec{E}|e^{-t^2/\tau^2}\langle f|\sqrt{\tfrac{\hbar}{2m\omega}}(a^\dagger + a)|i\rangle$$

$$= -eEe^{-t^2/\tau^2}\sqrt{\tfrac{\hbar}{2m\omega}}\left[\langle f|a^\dagger|i\rangle + \langle f|a|i\rangle\right]$$

d) $P = |c_n^{(1)}|^2$, now specifying $|f\rangle = |1\rangle$, $|i\rangle = |0\rangle$

$$V_{ni} = -eEe^{-t^2/\tau^2}\sqrt{\tfrac{\hbar}{2m\omega}}\left[\langle 1|a^\dagger|0\rangle + \cancel{\langle 1|a|0\rangle}^{\,0}\right]$$

$$= -eEe^{-t^2\tau^2}\sqrt{\tfrac{\hbar}{2m\omega}}$$

$$\hookrightarrow c_{10}^{(1)} = \frac{-i}{\hbar}\int_{-\infty}^{\infty} e^{-i\omega_{10}t'}\left(-eEe^{-t^2/\tau^2}\right)dt' \cdot \sqrt{\tfrac{\hbar}{2m\omega}}$$

$$= \frac{ieE}{\hbar}\sqrt{\frac{\hbar}{2m\omega}}\int_{-\infty}^{\infty} e^{-i\omega_{10}t'} e^{-t'^2/\tau^2}\,dt'$$

$$= \frac{ieE}{\hbar}\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{\pi}\tau \exp[-\omega_{10}^2\tau^2/4]\right)$$

$$\underline{P} = \frac{e^2E^2}{\hbar^2}\left(\frac{\hbar}{2m\omega}\right)\pi\tau \exp[-\omega_{10}^2\tau^2/2], \quad \omega_{10} = \frac{E_1^{(0)} - E_0^{(1)}}{\hbar}$$

PROBLEM 4: Two Particles in a 1D Box

Consider two noninteracting particles of mass m inside a 1D box,

$$V(x) = \begin{cases} 0 & , 0 < |x| < a \\ \infty & , \text{otherwise} \end{cases} .$$

Make sure to consider the spin part of the wavefunction in this problem.

a) Let n_1 and n_2 be the quantum numbers of particle 1 and 2 respectively. What are the wavefunctions of the single particle states for the each particle in the box? What are the single particle energies? (2 Points)

b) If the particles are distinguishable what is the two-particle wavefunction that describes the state? What is the energy? Write out explicitly the state (or states) and energies for the ground state and first excited states of the system. (2 Points)

c) If the two particles are identical spin 0 bosons what are the ground state and first excited state wavefunctions and energies? (2 Points)

d) If the two particles are identical spin 1/2 fermions what are the ground state and first excited state wavefunctions and energies? (2 Points)

e) Write down the Hamiltonian for the two particles in the box and show that when the particles are identical H commutes with the exchange operator. (2 Points)

#4 (cont.)

a) * Similarly, if n = odd: $A = 0$, $B = \sqrt{\frac{1}{a}}$

$\Rightarrow$ For any single particle: $\boxed{\psi(x) = \begin{cases} \sqrt{\frac{1}{a}} \sin\left(\frac{n\pi x}{2a}\right) & n = \text{even} \\ \sqrt{\frac{1}{a}} \cos\left(\frac{n\pi x}{2a}\right) & n = \text{odd} \end{cases}}$

$$k = \frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{2a}$$

$$\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}}$$

b) Assuming distinguishable particles, our two particle wave functions will be the product of the two single particle states, plus a spin function

$$\psi_{sys} = \psi_{n_1}\psi_{n_2}\psi_{spin}, \quad E_{sys} = \frac{(n_1^2+n_2^2)\pi^2\hbar^2}{2ma^2}$$

The ground state occurs when $n_1 = n_2 = 1$

$$\psi_{sys} = \frac{1}{a}\cos\left(\frac{\pi x_1}{2a}\right)\cos\left(\frac{\pi x_2}{2a}\right)$$

$$E = \frac{\pi^2\hbar^2}{ma^2}$$

The first excited state occurs when $(n_1 = 2, n_2 = 1)$ or $(n_1 = 1, n_2 = 2)$

$$\psi_{sys} = \frac{1}{a}\sin\left(\frac{\pi x_1}{a}\right)\cos\left(\frac{\pi x_2}{2a}\right) \qquad E = \frac{5\pi^2\hbar^2}{2ma^2}$$

or

$$\psi_{sys} = \frac{1}{a}\cos\left(\frac{\pi x_1}{2a}\right)\sin\left(\frac{\pi x_2}{a}\right) \qquad E = \frac{5\pi^2\hbar^2}{2ma^2}$$

c) Our spin function now becomes important. Bosons must have symmetric spin functions which we will denote ψ_{spin}^{sym}. Since our bosons are identical, and thus indistinguishable, it will be a superposition of the two possible single particle states

$\Rightarrow$ In the ground state, $E_{sys} = \frac{\pi^2\hbar^2}{ma^2}$

$$\psi_{sys} = A\left[\frac{1}{a}\cos\left(\frac{\pi x_1}{2a}\right)\cos\left(\frac{\pi x_2}{2a}\right) + \frac{1}{a}\cos\left(\frac{\pi x_1}{2a}\right)\cos\left(\frac{\pi x_2}{2a}\right)\right]$$

$$= \frac{2A}{a}\cos\left(\frac{\pi x_1}{2a}\right)\cos\left(\frac{\pi x_2}{2a}\right),$$ A is normalization constant

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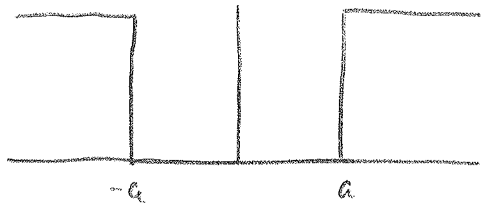
Quantum #4

a) For two non-interacting particles in a box, where

$$V(x) = \begin{cases} 0 & 0 < |x| < a \\ \infty & \text{otherwise} \end{cases}$$



$$H\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d^2\psi}{dx^2} = \frac{-\sqrt{2mE}}{\hbar}\psi$$

$$= -k^2\psi$$

$\hookrightarrow \psi = A\sin(kx) + B\cos(kx)$

* Our boundary conditions are $\psi(-a) = 0 = \psi(a)$

$$0 = A\sin(-ka) + B\cos(-ka)$$

$$0 = A\sin(ka) + B\cos(ka)$$

$\hookrightarrow$ Our trig functions will be 0 when $ka = \frac{n\pi}{2} \iff k = \frac{n\pi}{2a}$

$\sin\left(\frac{n\pi}{2}\right) = 0$ if $n =$ even $(0,2,4,$ etc$)$

$\cos\left(\frac{n\pi}{2}\right) = 0$ if $n =$ odd $(1,3,5,$ etc$)$

* if $n =$ even,

$$\psi = A(0) + B\cos\left(\frac{n\pi}{2}\right) \Rightarrow B = 0$$

$$1 = A^2\int_{-a}^{a}\sin^2\left(\frac{n\pi x}{2}\right)dx$$

$$1 = \frac{A^2}{2}\int_{-a}^{a}\left[1 - \cos\left(\frac{n\pi x}{2a}\right)\right]dx$$

$$1 = \frac{A^2}{2}\left[x - \sin\left(\frac{n\pi x}{a}\right)\right]\Big|_{-a}^{a}$$

$$1 = \frac{A^2}{2}\left[\left(a - \frac{1}{n\pi}\cancel{\sin\left(\frac{n\pi a}{a}\right)}^{0}\right) - \left(-a - \frac{1}{n\pi}\cancel{\sin\left(\frac{-n\pi a}{a}\right)}^{0}\right)\right]$$

$$1 = \frac{A^2}{2}[2a] \Rightarrow A = \sqrt{\frac{1}{a}}$$

#4 (cont)

c) $\Rightarrow$ In the first excited state, $E_{sys} = \frac{5\pi^2\hbar^2}{2ma^2}$

$$\psi_{sys} = A\left[\frac{1}{a}\sin\left(\frac{\pi x_1}{2a}\right)\cos\left(\frac{\pi x_2}{a}\right) + \frac{1}{a}\cos\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{2a}\right)\right]$$

d) With two identical spin ½ fermions, we need an antisymmetric spin function, denoted ψ_{spin}^{asym}, and an antisymmetric wave function

$\Rightarrow$ In the ground state, $E_{sys} = \frac{\pi^2\hbar^2}{2ma^2}$ (1 particle spin up, 1 spin down will violate exclusion principle)

$$\psi_{sys} = A\left[\frac{1}{a}\sin\left(\frac{\pi x_1}{2a}\right)\sin\left(\frac{\pi x_2}{2a}\right) - \frac{1}{a}\sin\left(\frac{\pi x_1}{2a}\right)\sin\left(\frac{\pi x_2}{2a}\right)\right]$$

$$= 0$$

Therefore, our ground state becomes $E_{sys} = \frac{5\pi^2\hbar^2}{2ma^2}$

$$\psi_{sys} = A\left[\frac{1}{a}\sin\left(\frac{\pi x_1}{2a}\right)\cos\left(\frac{\pi x_2}{a}\right) - \frac{1}{a}\cos\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{2a}\right)\right]$$

$\Rightarrow$ Now the first excited state occurs when $(n_1 = 1, n_2 = 3)$ or $(n_1 = 3, n_2 = 1)$. with $E_{sys} = \frac{5\pi^2\hbar^2}{ma^2}$

$$\psi_{sys} = A\left[\frac{1}{a}\sin\left(\frac{\pi x_1}{2a}\right)\sin\left(\frac{3\pi x_2}{2a}\right) - \frac{1}{a}\sin\left(\frac{3\pi x_1}{2a}\right)\sin\left(\frac{\pi x_2}{2a}\right)\right]$$

e) The Hamiltonian for the system is:

$$H = \frac{-\hbar^2}{2m}\left[\frac{d^2}{dx_1^2} + \frac{d^2}{dx_2^2}\right]$$

PROBLEM 5: Addition of angular momenta

Consider an electron. We know its orbital angular momentum $\ell = 1$ and the z component $m = 1/2$ of its total angular momentum j.

a) What are the possible values of j? (2 Points).

b) Write down the kets $|\ell = 1, \frac{1}{2}; j, m = \frac{1}{2}\rangle$ in terms of products of spin and orbital angular momentum states (3 Points)

c) Calculate the expectation value of the spin operator $\mathbf{S}$ in the state $|\ell = 1, \frac{1}{2}; j, m = \frac{1}{2}\rangle$. Consider all possible values of j. (3 Points).

d) The magnetic dipole moment of the electron is

$$\boldsymbol{\mu} = \frac{e}{2m_e c}(\mathbf{L} + 2\mathbf{S}),$$

with $\mathbf{L}$ the orbital angular momentum operator, e the electron charge, m_e the mass and c the speed of light. Calculate the expectation value of $\boldsymbol{\mu}$ in the states $|\ell = 1, \frac{1}{2}; j, m = \frac{1}{2}\rangle$. (2 Points)

Raising and lowering angular momentum operators:

$$J_{\pm}|j, m\rangle = \hbar\sqrt{(j \mp m)(j \pm m + 1)}|j, m \pm 1\rangle$$

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Quantum #5

a) Given an electron w/ $\ell = 1$, $m = 1/2$, we know that

$$|\ell - m| \leq j \leq |\ell + s|$$

$$|1 - 1/2| \leq j \leq |1 + 1/2|$$

$$1/2 \leq j \leq 3/2$$

$$\hookrightarrow j = \{1/2, 3/2\}$$

b) We must use Clebsh - Gordon coefficients, we start in the highest state and use the lowering operator

$$|\ell = 1, m = 1/2; 3/2, 3/2\rangle = |\ell = 1, m_\ell = 1\rangle \otimes |s = 1/2, m_s = 1/2\rangle$$

$$J_-|\ell = 1, m = 1/2; 3/2, 3/2\rangle = \hbar\sqrt{(\tfrac{3}{2}+\tfrac{3}{2})(3/2 - 3/2 + 1)}\ |1, 1/2; 3/2, 1/2\rangle$$

$$= \hbar\sqrt{3}$$

$$J_-|1,1\rangle \otimes |1/2, 1/2\rangle = J_-^L|1,1\rangle \otimes |1/2, 1/2\rangle + |1,1\rangle \otimes J_-^S|1/2, 1/2\rangle$$

$$= \sqrt{2}\hbar|1,0\rangle \otimes |1/2, 1/2\rangle + \hbar|1,1\rangle \otimes |1/2, -1/2\rangle$$

$$|1, 1/2; 3/2, 1/2\rangle = \frac{\sqrt{2}}{\sqrt{3}}\left[|1,0\rangle \otimes |1/2, 1/2\rangle\right] + \frac{1}{\sqrt{3}}\left[|1,1\rangle \otimes |1/2, -1/2\rangle\right]$$

To determine the $|1, 1/2; 1/2, 1/2\rangle$ state, we use the orthogonality condition

$$\langle 1, 1/2; 3/2, 1/2 | 1, 1/2; 1/2, 1/2\rangle = 0$$

letting $|1, 1/2; 1/2, 1/2\rangle = A\left[|1,0\rangle \otimes |1/2, 1/2\rangle\right] + B\left[|1,1\rangle \otimes |1/2, -1/2\rangle\right]$

where $A^2 + B^2 = 1$

$$\hookrightarrow 0 = A\cdot\sqrt{\tfrac{2}{3}} + B\sqrt{\tfrac{1}{3}}$$

$$-B\sqrt{\tfrac{1}{3}} = A\sqrt{\tfrac{2}{3}} \Rightarrow A = \frac{-B}{\sqrt{2}}$$

$$1 = \frac{B^2}{2} + B^2 \Rightarrow B = \sqrt{\tfrac{2}{3}},\ A = \frac{-1}{\sqrt{3}}$$

$$\hookrightarrow |1, 1/2; 1/2, 1/2\rangle = \frac{-1}{\sqrt{3}}|1,0\rangle \otimes |1/2, 1/2\rangle + \sqrt{\tfrac{2}{3}}|1,1\rangle \otimes |1/2, -1/2\rangle$$

#5 (cont.)

c)

PROBLEM 6: Variational approach

A particle with mass, m, moving in one dimension finds itself in a potential given by,

$$V = \infty \quad \text{for} \quad x < 0$$

and

$$V = \beta x^3 \quad \text{for} \quad x > 0$$

where β is a positive constant.

a) Find an approximation to the ground state energy, using the trial wavefunction

$$\Psi = 0 \quad \text{for} \quad x < 0$$

and

$$\Psi = Cxe^{-\alpha x} \quad \text{for} \quad x > 0.$$

where C and α are positive constants. (5 Points)

b) Would you expect the exact ground state energy to be less than your answer to part (a), or greater than it? Justify. (3 Points)

c) How would you go about finding an excited state in this system using the same approach? (2 Points)

Hint: $\int_0^\infty x^2 e^{-ax} = 2a^{-3}$, for $a > 0$.

Aug 2014

Quantum #6

a) The Variational principle states that $E_{gs} \leq \langle\psi|H|\psi\rangle = \langle H\rangle$ where $|\psi\rangle$ is a normalized trial wave function

$$\hookrightarrow H = \frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \beta x^3 = E\psi$$

$$V = \begin{cases} 0 & x < 0 \\ \beta x^3 & x \geq 0 \end{cases}$$

$$\psi = \begin{cases} Cxe^{-\alpha x} & x \geq 0 \\ 0 & x < 0 \end{cases}$$

* We first normalize our trial wave function, domain of interest is $[0, a)$

$$1 = C^2 \int_0^\infty x^2 e^{-2\alpha x}\,dx$$

* we know $\int_0^\infty x^2 e^{-ax} = 2a^{-3}$, $a > 0$

$$\hookrightarrow a = 2\alpha$$

$$1 = C^2 \cdot 2(2\alpha)^{-3}$$

$$1 = C^2 \cdot \frac{1}{4\alpha^3}$$

$$\hookrightarrow C = 2\alpha^{3/2}$$

$$\Rightarrow \psi(x) = \begin{cases} 2\alpha^{3/2} x e^{-\alpha x} & x \geq 0 \\ 0 & x < 0 \end{cases}$$

$$\langle H\rangle = \langle\psi|H|\psi\rangle$$

$$= \int_0^\infty 2\alpha^{3/2} x e^{-\alpha x}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \beta x^3\right) 2\alpha^{3/2} x e^{-\alpha x}\,dx$$

$$= \int_0^\infty 2\alpha^{3/2} x e^{-\alpha x}\left[-\frac{\hbar^2\alpha^{3/2}}{m}\frac{d^2(xe^{-\alpha x})}{dx^2} + 2\alpha^{3/2}\beta x^4 e^{-\alpha x}\right]dx$$

$$= \int_0^\infty 2\alpha^{3/2} x e^{-\alpha x}\left[-\frac{\hbar^2\alpha^{3/2}}{m}(\alpha^2 x - 2\alpha)e^{-\alpha x} + 2\alpha^{3/2}\beta x^4 e^{-\alpha x}\right]dx$$

$$= \int_0^\infty -\frac{2\alpha^3 x\hbar^2}{m}(\alpha^2 x - 2\alpha)e^{-2\alpha x} + 4\alpha^3\beta x^5 e^{-2\alpha x}\,dx$$

#6 (cont.)

a) $\langle H \rangle = \frac{-2\alpha^5\hbar^2}{m}\int_0^\infty x^2 e^{-2\alpha x}dx + \frac{4\alpha^4\hbar^2}{m}\int_0^\infty x e^{-2\alpha x}dx + 4\alpha^3\beta\int_0^\infty x^5 e^{-2\alpha x}dx$

* in general, $\int_0^\infty x^n e^{-bx} = \frac{n!}{b^{n+1}}$

$$= -\frac{2\alpha^5\hbar^2}{m}\left[\frac{2!}{(2\alpha)^3}\right] + \frac{4\alpha^4\hbar^2}{m}\left[\frac{1!}{(2\alpha)^2}\right] + 4\alpha^3\beta\left[\frac{5!}{(2\alpha)^6}\right]$$

$$= \frac{-4\alpha^5\hbar^2}{8\alpha^3 m} + \frac{4\alpha^4\hbar^2}{4\alpha^2 m} + \frac{4\alpha^3\beta\cdot 120}{64\alpha^6}$$

$$= \frac{-\alpha^2\hbar^2}{2m} + \frac{\alpha^2\hbar^2}{m} + \frac{30\beta}{4\alpha^3}$$

$$= \frac{\alpha^2\hbar^2}{2m} + \frac{15\beta}{2\alpha^3}$$

b) By definition, our $E_{gs} \le \langle H \rangle$. To prove this, we write our trial function as an expansion in eigenfunctions of H

$$|\psi\rangle = \sum_n c_n |\psi_n\rangle \quad \text{where} \quad H|\psi_n\rangle = E_n|\psi_n\rangle$$
$$|c_n|^2 = 1$$

$$\Rightarrow \langle H \rangle = \langle \psi | H | \psi \rangle$$

$$= \sum_{nm} \langle \psi_m | c_m^* H c_n | \psi_n \rangle$$

$$= \sum_{nm} c_m^* c_n \langle \psi_m | H | \psi_n \rangle$$

$$= \sum_{nm} c_m^* c_n E_n \langle \psi_m | \psi_n \rangle$$

$$= \sum_{nm} c_m^* c_n E_n \delta_{mn}$$

$$= \sum_n |c_n|^2 E_n$$

$\Rightarrow E_{gs} = \sum_n |c_n|^2 E_n$ if n is ground state, otherwise

$E_{gs} < \sum_n |c_n|^2 E_n$

#6 (cont.)

c) To get an upper bound on the first excited state, we need a wavefunction that is orthogonal to the ground state wave function ψ_{gs}. However, since this is difficult to know, an equivalent option is to use a trial wave function with a parity opposite to that of the potential. Then we proceed as before.