

Quantum Mechanics
Qualifying Exam - January 2015

Notes and Instructions

- There are 6 problems. Attempt them all as partial credit will be given.
- Write on only one side of the paper for your solutions.
- 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 your work to receive full credit.

Possibly useful formulas:

Spin Operator

$$\vec{S} = \frac{\hbar}{2} \vec{\sigma}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (1)$$

In spherical coordinates,

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

Problem 1: Solving the Harmonic Oscillator

Solving the differential equation form of the time-independent Schrödinger equation for the eigenstates of the harmonic oscillator Hamiltonian in 1D requires solving a second order differential equation. By using operator algebra, it is possible to simplify the solution to this problem.

The 1D harmonic oscillator is described by the Hamiltonian

$$H = \frac{P^2}{2m} + \frac{m}{2}\omega^2 X^2. \quad (1)$$

Define the unitless variables

$$x = \frac{X}{\lambda}, \quad p = \frac{\lambda}{\hbar}P, \quad \lambda = \sqrt{\frac{\hbar}{m\omega}}. \quad (2)$$

such that the Hamiltonian has the form

$$H = \frac{\hbar\omega}{2} (p^2 + x^2). \quad (3)$$

Note that x and p are conjugate observables, $[x, p] = i$

(a) [2 pt] Using the harmonic oscillator operators

$$\hat{a} = \frac{1}{\sqrt{2}}(x + ip), \quad \hat{a}^\dagger = \frac{1}{\sqrt{2}}(x - ip), \quad \hat{n} = \hat{a}^\dagger \hat{a}, \quad (4)$$

and their commutation relations, show that the Hamiltonian can be written as

$$H = \hbar\omega(\hat{n} + \frac{1}{2}). \quad (5)$$

(b) [2 pts] Define the eigenstates of the operator \hat{n} :

$$\hat{n}|n\rangle = n|n\rangle, \quad (6)$$

with n some (unitless) numbers. Use the operator commutation relations to show that

$$\begin{aligned} \hat{a}|n\rangle &= c(n)|n-1\rangle \\ \hat{a}^\dagger|n\rangle &= d(n)|n+1\rangle. \end{aligned} \quad (7)$$

Derive expressions for $c(n)$ and $d(n)$. Show your work.

(c) [3 pts] The potential, $V(x) = \frac{\hbar\omega}{2}x^2 \geq 0$ for all x . Explain why this implies that:

1. The eigenenergies of the Harmonic Oscillator must be positive
2. The eigenvalues of \hat{n} must be non-negative integers
3. There is a lowest eigenstate of \hat{n} , $|0\rangle$ defined by $\hat{a}|0\rangle = 0$.

(d) [2 pts] Show that results above define a first order differential equation in X that can be solved for the ground state harmonic oscillator wavefunction $\psi_0(X)$. Determine this equation and solve for this wavefunction.

(e) [1 pt] Use the result from (e) and the operators to determine the first excited state wavefunction for the harmonic oscillator, $\psi_1(X)$.

a) Given: $H = \frac{\hbar\omega}{2} (p^2 + x^2)$, $[x, p] = i$

$$a = \frac{1}{\sqrt{2}}(x + ip) \quad a^\dagger = \frac{1}{\sqrt{2}}(x - ip) \quad n = a^\dagger a$$

* Rewrite H in terms a, a^\dagger then

$$\begin{aligned} \Rightarrow \sqrt{2}a &= (x + ip) & \Leftrightarrow & \quad x = \frac{1}{\sqrt{2}}(a + a^\dagger) \\ \sqrt{2}a^\dagger &= (x - ip) & & \quad p = \frac{i}{\sqrt{2}}(a - a^\dagger) \end{aligned}$$

$$\begin{aligned} \Rightarrow H &= \frac{\hbar\omega}{2} \left(\left[\frac{-i}{\sqrt{2}}(a - a^\dagger) \right]^2 + \left[\frac{1}{\sqrt{2}}(a + a^\dagger) \right]^2 \right) \\ &= \frac{\hbar\omega}{2} \left(\frac{-1}{2}(aa - a^\dagger a - aa^\dagger + a^\dagger a^\dagger) + \frac{1}{2}(aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger) \right) \\ &= \frac{\hbar\omega}{2} (aa^\dagger + a^\dagger a) \\ &= \frac{\hbar\omega}{2} (a^\dagger a + 1 + a^\dagger a) \quad (\text{from } [a, a^\dagger] = 1) \\ &= \hbar\omega(n + 1/2) \checkmark \end{aligned}$$

b) * Remember that $[n, a] = -a$, $[n, a^\dagger] = a^\dagger$

\Rightarrow Solve by using the above commutator relations

$$\begin{aligned} n(a|n\rangle) &= (an - a)|n\rangle \\ &= a(n-1)|n\rangle \\ &= (n-1)(a|n\rangle) \quad \Rightarrow a|n\rangle = c_n |n-1\rangle \end{aligned}$$

$$\begin{aligned} n(a^\dagger|n\rangle) &= (a^\dagger n + a^\dagger)|n\rangle \\ &= a^\dagger(n+1)|n\rangle \\ &= (n+1)(a^\dagger|n\rangle) \quad \Rightarrow a^\dagger|n\rangle = d_n |n+1\rangle \end{aligned}$$

\Rightarrow Determine c_n and d_n through normalization

$$\langle n|a^\dagger a|n\rangle = |c_n|^2 \langle n-1|n-1\rangle$$

$$n \langle n|n\rangle = |c_n|^2$$

$$n = |c_n|^2 \Rightarrow \boxed{c_n = \sqrt{n}}$$

#1(cont.)

$$b) \quad \langle n | a a^\dagger | n \rangle = |d_n|^2 \langle n+1 | n+1 \rangle$$

$$\langle n | a^\dagger a + 1 | n \rangle = |d_n|^2$$

$$(n+1) \langle n | n \rangle = |d_n|^2$$

$$n+1 = |d_n|^2 \Rightarrow d_n = \sqrt{n+1}$$

- c) ① Given a potential $V(x) = \frac{1}{2} \hbar \omega x^2 \geq 0$ for all x and combined with the fact that $T \geq 0$ (since kinetic energy can never be negative), then $(H = T + V) \geq 0$ at all times, thus its eigenenergies must also be positive

② We can rewrite our potential as: $V = \frac{1}{2} \hbar \omega \left(\frac{a + a^\dagger}{\sqrt{2}} \right)^2$

$$\Rightarrow V = \frac{\hbar \omega}{4} (aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger)$$

$$V|n\rangle = \frac{\hbar \omega}{4} (aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger)|n\rangle$$

$$= \frac{\hbar \omega}{4} [\sqrt{n(n-1)}|n-2\rangle + \sqrt{n+1}\sqrt{n+1}|n\rangle + \sqrt{n}\sqrt{n}|n\rangle + \sqrt{(n+1)(n+2)}|n+2\rangle]$$

$$= \frac{\hbar \omega}{4} [\sqrt{n(n-1)}|n-2\rangle + (2n+1)|n\rangle + \sqrt{(n+1)(n+2)}|n+2\rangle]$$

* For the above equation to be greater than or equal to 0, n must also be greater than or equal to 0

- ③ In order for the above to be true $a|0\rangle = 0$ because $n \geq 0$. Following our work from part b

$$n(a|0\rangle) = (an - a)|0\rangle$$

$$= a(0-1)|0\rangle$$

$$= -a|0\rangle = c_n|-1\rangle$$

$$\langle 0 | -a^\dagger - a | 0 \rangle = |c_n|^2 \langle -1 | -1 \rangle$$

$$0 \langle 0 | 0 \rangle = |c_n|^2 \langle -1 | -1 \rangle$$

$$0 = |c_n|^2 \langle -1 | -1 \rangle$$

$$\hookrightarrow \langle -1 | -1 \rangle = 0$$

#1 (cont.)

d) If we let $\psi_0 = \psi_0$

$$a \psi_0 = 0$$

$$\frac{1}{\sqrt{2}} (x + ip) \psi_0 = 0$$

$$\frac{1}{\sqrt{2}} \left(\frac{1}{\lambda} x + i \frac{\lambda}{\hbar} p \right) \psi_0 = 0$$

$$\frac{1}{\sqrt{2}} \left(\frac{1}{\lambda} x + i \frac{\lambda}{\hbar} \left(-i \hbar \frac{\partial}{\partial x} \right) \right) \psi_0 = 0$$

$$\frac{1}{\sqrt{2}} \left(\frac{1}{\lambda} x + \lambda \frac{\partial}{\partial x} \right) \psi_0 = 0$$

$$\frac{1}{\lambda} x \psi_0 = -\lambda \frac{\partial \psi_0}{\partial x}$$

$$\int x \partial x = \int -\lambda^2 \frac{\partial \psi_0}{\psi_0}$$

$$\frac{1}{2\lambda^2} x^2 + C = \ln(\psi_0)$$

$$\exp \left[\frac{-x^2}{2\lambda^2} + C \right] = \psi_0$$

$$\hookrightarrow \psi_0 = C \exp \left[\frac{m\omega x^2}{2\hbar} \right]$$

* Normalizing our wavefunction

$$1 = \int |\psi_0|^2 dx$$

$$1 = C^2 \int \left| \exp \left[\frac{m\omega}{2\hbar} x^2 \right] \right|^2 dx$$

$$1 = C^2 \int \exp \left[\frac{m\omega}{\hbar} x^2 \right] dx$$

$$1 = C^2 \sqrt{\frac{\pi \hbar}{m\omega}}$$

$$\hookrightarrow C = \left(\frac{m\omega}{\pi \hbar} \right)^{1/4}$$

$$\Rightarrow \psi_0 = \left(\frac{m\omega}{\pi \hbar} \right)^{1/4} \exp \left[\frac{m\omega}{2\hbar} x^2 \right]$$

#1 (cont.)

e) * Following a similar progression to part d

$$|1\rangle = \psi_1 = a^\dagger |0\rangle$$

$$\psi_1 = \frac{1}{\sqrt{2}} (x - c p) \psi_0$$

$$= \frac{1}{\sqrt{2}} \left(\frac{x}{\lambda} - i \frac{\lambda}{\hbar} (-i \hbar \frac{\partial}{\partial x}) \right) \psi_0$$

$$= \frac{1}{\sqrt{2}} \left(\frac{x}{\lambda} - \lambda \frac{\partial}{\partial x} \right) \psi_0$$

$$= \frac{1}{\sqrt{2}} \left(\sqrt{\frac{m\omega}{\hbar}} x - \sqrt{\frac{\hbar}{m\omega}} \frac{\partial}{\partial x} \right) \left[\left(\frac{m\omega}{\pi \hbar} \right)^{1/4} \exp \left[-\frac{m\omega}{2\hbar} x^2 \right] \right]$$

$$= \frac{1}{\sqrt{2}} \left(\sqrt{\frac{m\omega}{\hbar}} x \psi_0 - \sqrt{\frac{\hbar}{m\omega}} \left(\frac{m\omega}{\pi \hbar} \right)^{1/4} \left(-x \frac{m\omega}{\hbar} \right) \exp \left[-\frac{m\omega}{2\hbar} x^2 \right] \right)$$

$$= \frac{1}{\sqrt{2}} \left(\sqrt{\frac{m\omega}{\hbar}} x \psi_0 + \sqrt{\frac{m\omega}{\hbar}} x \psi_0 \right)$$

$$= \sqrt{\frac{2m\omega}{\hbar}} x \left(\frac{m\omega}{\pi \hbar} \right)^{1/4} \exp \left[-\frac{m\omega}{2\hbar} x^2 \right]$$

Problem 2: Angular Momentum States

Consider the electron in a hydrogen atom in the presence of a homogeneous magnetic field $\mathbf{B} = B\hat{\mathbf{z}}$. In this problem, ignore the electron spin and only consider the orbital angular momentum. The Hamiltonian of the system is

$$\mathcal{H} = \mathcal{H}_0 - \omega L_z, \quad (1)$$

where \mathcal{H}_0 is the Hamiltonian for the hydrogen atom, $\omega \equiv |e|B/2m_e c$, and L_z is the angular momentum operator along the z direction. The eigenstates $|n, \ell, m\rangle$ and eigenvalues $E_n^{(0)}$ of the unperturbed hydrogen atom are to be considered as known. Assume that, initially (at $t = 0$) the system is in the state

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}} (|2, 1, -1\rangle - |2, 1, 1\rangle). \quad (2)$$

- (a) [1 pt] Write down the time-dependent state for this atom, $|\psi(t)\rangle$, given the initial state and the full Hamiltonian.
- (b) [2 pts] Calculate the probability of finding the atom at some later time $t > 0$ in the state

$$|2p_y\rangle = \frac{1}{\sqrt{2}} (|2, 1, -1\rangle + |2, 1, 1\rangle). \quad (3)$$

When is the probability equal to 1?

- (c) [3 pts] Define the state $|\mathbf{e}_\phi\rangle$ defined by

$$(\mathbf{e}_\phi \cdot \mathbf{L}) |\mathbf{e}_\phi\rangle = \hbar |\mathbf{e}_\phi\rangle, \quad \mathbf{L}^2 |\mathbf{e}_\phi\rangle = 2\hbar^2 |\mathbf{e}_\phi\rangle. \quad (4)$$

\mathbf{e}_ϕ is a unit vector in the $x - y$ plane, $\mathbf{e}_\phi = \cos(\phi)\mathbf{e}_x + \sin(\phi)\mathbf{e}_y$.

This state has quantum number $\ell = 1$ and angular momentum projection along the direction \mathbf{e}_ϕ equal to $+\hbar$. Solve for the state $|\mathbf{e}_\phi\rangle$ in the basis of states $|2, 1, m\rangle$, with $m = \pm 1, 0$.

- (d) [2 pts] Calculate the time-dependent probability of finding the system in the state $|\mathbf{e}_\phi\rangle$, if it starts in the state $|\psi(0)\rangle$ above, and show that this is a periodic function of time. Calculate the times when the probability is maximum and minimum.
- (e) [2 pts] If the electron starts in the state $|\psi(0)\rangle$, calculate the expectation value of the magnetic dipole

$$\langle \vec{\mu} \rangle(t) = \frac{e}{2m_e c} \langle \mathbf{L} \rangle(t), \quad \mathbf{L} = L_x \mathbf{e}_x + L_y \mathbf{e}_y + L_z \mathbf{e}_z \quad (5)$$

as a function of time.

Hint: It will be useful to use:

$$\begin{aligned} J_\pm &= J_x \pm iJ_y \\ J_\pm |j, m\rangle &= \hbar \sqrt{j(j+1) - m(m \pm 1)} |j, m \pm 1\rangle \end{aligned} \quad (6)$$

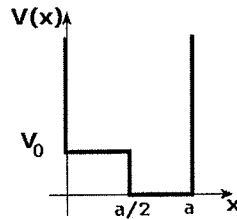
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Quantum #2

Problem 3: Double Step Potential

Consider a single particle of mass m in a one dimensional well of width a and a potential, $V(x)$, given by:

$$V(x) = \begin{cases} \infty, & x < 0 \\ V_0, & 0 < x < \frac{a}{2} \\ 0, & \frac{a}{2} < x < a \\ \infty, & x > a \end{cases} \quad (1)$$



In this question, you will consider the special cases where this potential well has a bound state at the energy $E = V_0$. There are only certain values of V_0 and a where this will happen.

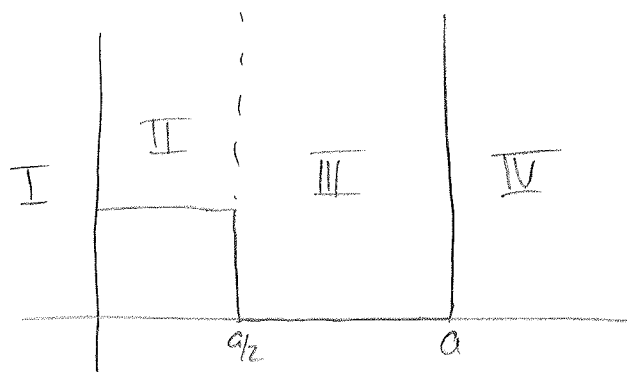
In this problem, use the constant

$$k = \sqrt{\frac{2mV_0}{\hbar^2}} \quad (2)$$

- [2 pts] For the energy $E = V_0$ in this potential, determine the general eigenfunction solutions to the time-independent Schrödinger equation in all regions of x . Show your work.
- [3 pts] Apply boundary conditions to determine relationships between the constants you introduced in writing the wave functions in part (a).
- [2 pts] From your results above, derive a transcendental equation that gives the values of V_0 where there is an energy eigenstate with $E = V_0$, for a fixed well width a . This equation will have the form $z = f(z)$ with $z = k\frac{a}{2}$. Plot this function and determine a relationship between the first energy V_0 that satisfies this equation and the bound state energies of a square well of width a .
- [2 pts] Qualitatively sketch the wave function that corresponds to the smallest value of V_0 that satisfies the transcendental equation from part (c), for a fixed value of a .
- [1 pt] Finally, consider the case where the width of the well is fixed but the potential step, V_0 , can be changed. There are an infinite number of possible values of V_0 where the well contains an energy eigenstate with $E = V_0$. Describe, qualitatively, the changes in the wavefunctions of these eigenstates as V_0 gets larger.

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Quantum #3



a) $H\psi_i = E\psi_i$

* In regions I + IV: $\psi_I = 0 = \psi_{IV}$ (due to infinite potential)

* In region III: $-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E\psi$

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{2mE}{\hbar^2} \psi$$

* if $k = \sqrt{\frac{2mV_0}{\hbar^2}}$ ($E = V_0$ as stated in problem)

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 \psi$$

$$\hookrightarrow \psi_{III}(x) = Ae^{-ikx} + Be^{ikx}$$

* In region II: $-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi = E\psi$

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

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

\hookrightarrow let $k = \sqrt{\frac{2m(E - V)}{\hbar^2}}$, $E = V_0$ as stated in problem

$$\frac{\partial^2 \psi}{\partial x^2} = 0$$

$$\hookrightarrow \psi_{II} = Cx + D$$

#3(cont.)

b) * Remember, our two boundary conditions are that: ψ is continuous

$\frac{d\psi}{dx}$ is continuous where $V \neq \infty$

$$0 = C(0) + D$$

$$\rightarrow \boxed{D = 0}$$

$$0 = Ae^{-ika} + Be^{ika}$$

$$= A + Be^{2ika}$$

$$\rightarrow \boxed{A = -Be^{2ika}}$$

$$C\left(\frac{a}{2}\right) = -Be^{3ika/2} + Be^{ika/2}$$

$$C = \frac{2B}{a}(e^{ika/2} - e^{3ika/2})$$

$$C = ikA(e^{ika/2} + e^{3ika/2})$$

Problem 4: Finite Quantum System

Consider a quantum system that can be described by three basis states, $|n\rangle$, $n = 1, 2, 3$, and the Hamiltonian in this basis:

$$H = \frac{\hbar\omega}{2} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & i \\ 0 & -i & 1 \end{pmatrix} \quad (1)$$

- (a) [3 pts] Solve for the energy eigenvalues and eigenstates of this system.
- (b) [2 pts] If the system starts in the state

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}} (|1\rangle + |2\rangle) \quad (2)$$

determine the time-dependence of the state $|\psi(t)\rangle$. You may write your answer in terms of either the states $|n\rangle$ or the eigenstates you found in part (a).

- (c) [3 pts] Calculate the time dependent probabilities for measuring the system to be in each of the states $|1\rangle$, $|2\rangle$, and $|3\rangle$, if the system starts in the state given in part (b). Explain why the different states can or cannot be measured and the frequency of the oscillations you found.
- (d) [2 pts] Finally, assume that the states $|n\rangle$ are the eigenstates of some observable O where

$$O|n\rangle = (-1)^n |n\rangle \quad (3)$$

If, again, the system starts in the state given in part (b), what is the time dependent expectation value of O , $\langle O \rangle(t)$?

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Quantum #4

$$a) H = \frac{\hbar\omega}{2} \begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & i \\ 0 & -i & 1 \end{bmatrix}$$

* Solving eigenvalue equation $\det(H - \lambda \mathbb{I}) = 0$

$$\begin{vmatrix} 2-\lambda & 0 & 0 \\ 0 & 1-\lambda & i \\ 0 & -i & 1-\lambda \end{vmatrix} = 0 = (2-\lambda)[(1-\lambda)^2 - (-i)(i)]$$

$$\Rightarrow 0 = (2-\lambda)[(1-\lambda)^2 - 1] \\ = (2-\lambda)[(1-\lambda)-1][(1-\lambda)+1]$$

$$\hookrightarrow \lambda = 2, 2, 0$$

* Solving eigenvector equation: $H\vec{x} = \lambda\vec{x}$

Case $\lambda = 0$:

$$2x_1 = 0$$

$$x_2 + ix_3 = 0 \rightarrow x_2 = -ix_3$$

$$-ix_2 + x_3 = 0 \rightarrow x_3 = ix_2$$

$$\rightarrow \vec{x} = \begin{bmatrix} 0 \\ -i \\ 1 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}$$

Case $\lambda = 2$

$$2x_1 = 2x_1$$

$$x_2 + ix_3 = 2x_2 \rightarrow ix_3 = x_2$$

$$-ix_2 + x_3 = 2x_3 \rightarrow -ix_2 = x_3$$

$$\vec{x} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \text{ or } \begin{bmatrix} 0 \\ i \\ 1 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}$$

b) * Proceed according to: $|1\rangle = \langle 1, 0, 0 \rangle, \lambda_1 = 2$

$$|2\rangle = \frac{1}{\sqrt{2}} \langle 0, i, 1 \rangle, \lambda_2 = 2$$

$$|3\rangle = \frac{1}{\sqrt{2}} \langle 0, -i, 1 \rangle, \lambda_3 = 0$$

* for rest of problem

$$\Rightarrow |\psi(0)\rangle = \frac{1}{\sqrt{2}} (|1\rangle + |2\rangle)$$

$$|\psi(t)\rangle = U(t, 0) |\psi(0)\rangle, \text{ where } U(t, 0) = e^{-iHt/\hbar}$$

$$= e^{-iHt/\hbar} \left(\frac{1}{\sqrt{2}} [|1\rangle + |2\rangle] \right)$$

$$= \frac{1}{\sqrt{2}} e^{-i2t/\hbar} (|1\rangle + |2\rangle)$$

#4 (cont.)

c) We want to calculate $|\langle n | \psi(t) \rangle|^2$ where $n \in \{1, 2, 3\}$

$$\begin{aligned} & |\langle 1 | \frac{1}{\sqrt{2}} e^{-iEt/\hbar} (|1\rangle + |2\rangle) |^2 \\ &= \frac{1}{2} |\langle 1 | 1 \rangle + \langle 1 | 2 \rangle|^2 \\ &= \frac{1}{2} \end{aligned}$$

$$\begin{aligned} & |\langle 3 | \frac{1}{\sqrt{2}} e^{-iEt/\hbar} (|1\rangle + |2\rangle) |^2 \\ &= \frac{1}{2} |\langle 3 | 1 \rangle + \langle 3 | 2 \rangle|^2 \\ &= 0 \end{aligned}$$

$$\begin{aligned} & |\langle 2 | \frac{1}{\sqrt{2}} e^{-iEt/\hbar} (|1\rangle + |2\rangle) |^2 \\ &= \frac{1}{2} |\langle 2 | 1 \rangle + \langle 2 | 2 \rangle|^2 \\ &= \frac{1}{2} \end{aligned}$$

\Rightarrow Oscillations will only occur if $|2\rangle$ has $\lambda = 0$
as this will prevent $e^{-iEt/\hbar} e^{iEt/\hbar} = 1$ term
from forming. In an abstract notation, you would
find oscillations with frequency $\frac{1}{\hbar}(\lambda_i - \lambda_j)$ where
 $i, j \in \{1, 2, 3\}$ and $i \neq j$

d) * Expectation values are by definition time-independent

$$\Rightarrow |\psi(0)\rangle = \frac{1}{\sqrt{2}} (|1\rangle + |2\rangle)$$

$$\begin{aligned} \langle O(t) \rangle &= \langle \psi(0) | U^\dagger O U | \psi(0) \rangle \\ &= \frac{1}{2} [(\langle 1 | + \langle 2 |) U^\dagger O U (|1\rangle + |2\rangle)] \\ &= \frac{1}{2} [\langle 1 | U^\dagger O U | 1 \rangle + \langle 1 | U^\dagger O U | 2 \rangle + \langle 2 | U^\dagger O U | 1 \rangle + \langle 2 | U^\dagger O U | 2 \rangle] \\ &= \frac{1}{2} [\langle 1 | 0 | 1 \rangle + \langle 1 | 0 | 2 \rangle + \langle 2 | 0 | 1 \rangle + \langle 2 | 0 | 2 \rangle] \\ &= \frac{1}{2} [(-1)^1 \cdot 1 + (-1)^2 \cdot 2 + (-1)^1 \cdot 1 + (-1)^2 \cdot 4] \\ &= \frac{1}{2} [-1 + 2 - 1 + 2] \\ &= 1 \end{aligned}$$

* See note from part e about oscillatory term if states $|2\rangle$ and $|3\rangle$ are mislabelled.
In the context of this problem, $e^{-iEt/\hbar}$ term introduced in cross terms

$$\hookrightarrow \langle O(t) \rangle = \frac{1}{2} [1 + e^{-iEt/\hbar}]$$

Problem 5: Interaction Picture of Quantum Mechanics

The “Interaction Picture” of quantum mechanics is in some ways in-between the Schrödinger formulation and the Heisenberg formulation.

Consider a system with the Hamiltonian $H = H_0 + V(t)$ where H_0 is independent of time and $V(t)$ may or may not be time dependent. The Interaction Picture is defined by the transformation of the Schrödinger states:

$$\begin{aligned} |\psi\rangle_I &= U_0^{-1} |\psi\rangle_S \\ U_0 &= e^{-\frac{i}{\hbar}(t-t_0)H_0}. \end{aligned} \quad (1)$$

The subscripts I and S refer to the Interaction Picture and Schrödinger Picture respectively. t_0 is a time when the pictures coincide, and we will set $t_0 = 0$ for this problem.

- (a) [1 pt] Show that U_0 is a unitary operator. Why is it important for the transformation between pictures be unitary?
- (b) [3 pts] The transformation between $|\psi\rangle_S$ and $|\psi\rangle_I$ implies that there is also a transformation of the observables between the pictures. If A_S and A_I are operators for an observable in the Schrödinger and Interaction pictures respectively, derive the relation between A_S and A_I . Show that this implies that H_0 is the same in the two pictures.
- (c) [3 pts] Derive the differential equation that determines the time dependence of the Interaction Picture states, $|\psi(t)\rangle_I$. Be sure to show and explain your work. Explain why the Interaction Picture may be particularly useful when $V(t)$ is “small”.
- (d) [1 pt] Define the eigenstates of H_0 to be

$$H_0|\lambda\rangle_S = E_\lambda|\lambda\rangle_S \quad (2)$$

Show that if $V(t) = 0$, the Interaction Picture energy eigenstates $|\lambda\rangle_I$ are equal to $|\lambda(t=0)\rangle_S$ and independent of time.

- (e) [2 pts] Consider a potential of the form

$$V(t) = 0, \quad t \leq 0 \quad V(t) \neq 0, \quad t > 0 \quad (3)$$

The system is in a state $|\psi_0\rangle_I$ for $t < 0$. For $t > 0$ the Interaction Picture state will depend on time. It can be expanded as:

$$|\psi(t)\rangle_I = \sum_{\lambda} c_{\lambda}(t) |\lambda(0)\rangle_I \quad (4)$$

In this expression, $c_{\lambda}(t)$ are time-dependent expansion coefficients for the state and $|\lambda(0)\rangle_I$ is the complete set of time-independent eigenstates of H_0 in the interaction picture.

Use the time dependence found in part (c) to derive a set of coupled equations relating $c_{\lambda}(t)$ and $\partial_t c_{\lambda}(t)$.

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Quantum #5

a) An operator is unitary if: $U^\dagger U = \mathbb{I}$

$$\rightarrow U = \exp\left[-\frac{i(t-t_0)H_0}{\hbar}\right]$$

$$U^\dagger = \exp\left[\frac{i(t-t_0)H_0}{\hbar}\right]$$

$$U^\dagger U = \exp\left[\frac{i(t-t_0)H_0}{\hbar}\right] \exp\left[-\frac{i(t-t_0)H_0}{\hbar}\right]$$

$$= \mathbb{I} \quad \checkmark$$

Our transformation must be a unitary operator b/c it preserves lengths of vectors, as well as the angles b/w them

b) This transformation is best seen in terms of an expectation value. In the Schrödinger picture:

$$\langle A \rangle = \langle \psi | A_S | \psi \rangle_S$$

Since we can only multiply by 1 and we want $|\psi\rangle_I = U_0^{-1} |\psi\rangle_S$

$$= \langle \psi | U_0 U_0^{-1} A_S U_0 U_0^{-1} | \psi \rangle_S$$

$$= \langle \psi | U_0^{-1} A_S U_0 | \psi \rangle_I$$

$$\rightarrow U_0^{-1} A_S U_0 = A_I$$

*Not sure I've fully answered this part

$$c) |\psi\rangle_I = \exp\left[\frac{i(t-t_0)H_0}{\hbar}\right] |\psi\rangle_S$$

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle_I = i\hbar \frac{\partial}{\partial t} \left(\exp\left[\frac{i(t-t_0)H_0}{\hbar}\right] |\psi\rangle_S \right)$$

$$= i\hbar \left(\frac{H_0}{i\hbar} \exp\left[\frac{i(t-t_0)H_0}{\hbar}\right] |\psi\rangle_S + \left[\frac{i(t-t_0)H_0}{\hbar} \right] \frac{\partial}{\partial t} |\psi\rangle_S \right)$$

$$= -H_0 \exp\left[\frac{i(t-t_0)H_0}{\hbar}\right] |\psi\rangle_S + (H_0 + V) |\psi\rangle_S \exp\left[\frac{i(t-t_0)H_0}{\hbar}\right]$$

$$= V \exp\left[\frac{i(t-t_0)H_0}{\hbar}\right] |\psi\rangle_S$$

$$= V |\psi\rangle_I$$

#5 (cont.)

$$c) i\hbar \frac{\partial}{\partial t} \langle n | \psi \rangle_I = \langle n | V | \psi \rangle_I$$

$$i\hbar \frac{\partial}{\partial t} c_n(t) = \sum_m \langle n | V | m \rangle \langle m | \psi \rangle_I$$

$$= \sum_m c_m V_{nm}$$

expanding $c_n(t)$ as $c_n^{(0)}(t) + \lambda c_n^{(1)}(t) + \dots$

$$i\hbar \frac{\partial}{\partial t} (c_n^{(0)}(t) + \lambda c_n^{(1)}(t) + \dots) = \sum_m (c_m^{(0)}(t) + \lambda c_m^{(1)}(t))$$

Problem 6: Perturbations in a 2D well

Consider a spinless particle of mass m and charge q confined to a hard-walled square well (in two dimensions) with sides of length L . The potential can be written:

$$\begin{aligned} V(x, y) &= 0, & -\frac{L}{2} \leq x \leq \frac{L}{2}, & -\frac{L}{2} \leq y \leq \frac{L}{2} \\ V(x, y) &= \infty & \text{otherwise} \end{aligned}$$

- (a) [2 pts] Write down the eigenenergies, eigenstates, and degeneracies of the first three energy levels for this well. You do not have to solve for these explicitly, but you must explain and justify how you obtained these results.
- (b) [2 pts] Consider applying a constant electric field in the x -direction to this system,

$$\vec{E} = E_0 \hat{e}_x \tag{1}$$

Assuming that E_0 is small, determine the first order shift in the energies for the ground state and first excited states. Be sure to show your work.

- (c) [3 pts] The second-order, in E_0 , energy shift of the ground state can be written in terms of a sum. Write down an expression for this sum using the general form for the eigenstates you determined in part (a). Calculate an approximate value for this energy shift by solving for the largest term in the sum. Your answer should be in terms of the parameters given in the problem, and fundamental constants.
- (d) [1 pt] Considering the sum you wrote down in part (c), what is the next largest term that will contribute a non-zero value to the sum? Explain your answer, but you do not need to compute this term.
- (e) [2 pts] Finally, instead of an electric field, consider the effect of a localized perturbation:

$$V(x, y) = V_0 L^2 \delta(x - x_0) \delta(y - y_0) \tag{2}$$

where (x_0, y_0) is some point in the well. Write down an expression for the first order energy shift for the ground state, showing how the energy shift depends on the position of the perturbation (x_0, y_0) .

Determine a position for the perturbation where the ground state energy changes, but the first excited state does not.

Determine a position for the perturbation that splits the degeneracy of the first excited state.

Jan 2015

Quantum #6

a) For a square well with walls at $[-\frac{1}{2}, \frac{1}{2}]$, our general wavefunctions and energies are:

$$\psi(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) & n = \text{even} \\ \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi x}{L}\right) & n = \text{odd} \end{cases}$$

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

Thus for a 2-D well, our wavefunctions/energies become:

$$\psi_{n_x n_y}(x, y) = \psi_{n_x}(x) \psi_{n_y}(y) \quad \text{where } \psi_{n_i}(i) \text{ is as above}$$

$$E_{n_x n_y} = \frac{(n_x^2 + n_y^2) \pi^2 \hbar^2}{2mL^2}$$

Our first three energy levels will be:

$$\textcircled{1} \quad n_x = 1, n_y = 1 \Rightarrow E_{11} = \frac{2\pi^2 \hbar^2}{2mL^2} \quad 9$$

$$\psi_{11} = \frac{2}{L} \cos\left(\frac{\pi x}{L}\right) \cos\left(\frac{\pi y}{L}\right) \quad 1$$

$$\textcircled{2} \quad n_x = 1, n_y = 2 \Rightarrow E_{12} = E_{21} = \frac{5\pi^2 \hbar^2}{2mL^2}$$

or

$$n_x = 2, n_y = 1$$

$$\psi_{12} = \frac{2}{L} \cos\left(\frac{\pi x}{L}\right) \sin\left(\frac{2\pi y}{L}\right) \quad 2$$

$$\psi_{21} = \frac{2}{L} \sin\left(\frac{2\pi x}{L}\right) \cos\left(\frac{\pi y}{L}\right)$$

$$\textcircled{3} \quad n_x = 2, n_y = 2 \Rightarrow E_{22} = \frac{8\pi^2 \hbar^2}{2mL^2}$$

$$\psi_{22} = \frac{2}{L} \sin\left(\frac{2\pi x}{L}\right) \sin\left(\frac{2\pi y}{L}\right) \quad 1$$

#6 (cont.)

b) Applying a constant E field $\vec{E} = E_0 \hat{x}$, yields a potential $V(x,y) = qE_0 x$

The equation that determines the first order energy correction is:

$$\Delta E_{n_x n_y}^{(1)} = \langle n_x n_y | V | n_x n_y \rangle$$

$$\Rightarrow \Delta E_{11}^{(1)} = \langle 1, 1 | qE_0 x | 1, 1 \rangle$$

$$= \int_{-L/2}^{L/2} dy \int_{-L/2}^{L/2} dx \left(\frac{2}{L}\right)^2 \cos^2\left(\frac{\pi x}{L}\right) \cos^2\left(\frac{\pi y}{L}\right) qE_0 x$$

$$= \int_{-L/2}^{L/2} qE_0 \cos^2\left(\frac{\pi y}{L}\right) dy \int_{-L/2}^{L/2} x \cos^2\left(\frac{\pi x}{L}\right) dx \cdot \left(\frac{2}{L}\right)^2$$

$$= \frac{4qE_0}{L^2} \int_{-L/2}^{L/2} \cos^2\left(\frac{\pi y}{L}\right) dy \left[\frac{x^2}{4} + \frac{x \sin\left(\frac{2\pi x}{L}\right)}{4(\pi/L)} + \frac{\cos\left(\frac{2\pi x}{L}\right)}{8(\pi/L)^2} \right] \Big|_{-L/2}^{L/2}$$

$$= \frac{4qE_0}{L^2} \int_{-L/2}^{L/2} \cos^2\left(\frac{\pi y}{L}\right) dy \left[\frac{(L/2)^2}{4} + \frac{L/2 \sin(\pi)}{4(\pi/L)} + \frac{\cos(\pi)}{8\pi^2/L^2} - \left(\frac{(-L/2)^2}{4} + \frac{-L/2 \sin(-\pi)}{4(\pi/L)} + \frac{\cos(-\pi)}{8\pi^2/L^2} \right) \right]$$

$$= \frac{4qE_0}{L^2} \int_{-L/2}^{L/2} \cos^2\left(\frac{\pi y}{L}\right) dy \left(\frac{L^2}{16} - \frac{L^2}{8\pi^2} - \left(\frac{L^2}{16} - \frac{L^2}{8\pi^2} \right) \right)$$

$$= 0$$

$$\Rightarrow \Delta E_{21}^{(1)} = \Delta E_{12}^{(1)}$$

$$= \langle 1, 2 | V | 1, 2 \rangle$$

$$= qE_0 \int_{-L/2}^{L/2} dy \int_{-L/2}^{L/2} \left(\frac{2}{L}\right)^2 \cos^2\left(\frac{\pi x}{L}\right) \sin^2\left(\frac{2\pi y}{L}\right) x dx$$

$$= qE_0 \int_{-L/2}^{L/2} \sin^2\left(\frac{2\pi y}{L}\right) dy \int_{-L/2}^{L/2} x \cos^2\left(\frac{\pi x}{L}\right) dx \cdot \frac{4}{L^2}$$

same as above, equals 0

$$= 0$$

#6 (cont.)

c) We know that the second order energy correction is given by:

$$\begin{aligned}\Delta E^{(2)} &= \sum_{k \neq n} \frac{|\langle k | V | n \rangle|^2}{E_n^{(0)} - E_k^{(0)}} \\ &= \sum_{k \neq n} \frac{\left| \int_{-L/2}^{L/2} dy \int_{-L/2}^{L/2} dx \, q E_0 \psi_{k_x k_y}^* \psi_{n_x n_y} \right|^2}{(n_x^2 + n_y^2) - (k_x^2 + k_y^2) \cdot \frac{\pi^2 \hbar^2}{2mL^2}}\end{aligned}$$

* Note that $\psi_{k_x k_y}^*$ and $\psi_{n_x n_y}$ will vary based on the values of the x-y states.

* Parity says that only odd functions will be non-zero over symmetric bounds, therefore since $n = (n_x=1, n_y=1)$ always yields an even function, our second order correction will always be 0 as even \cdot odd = even