

Quantum Mechanics

Qualifying Exam – August 2006

Notes and Instructions:

- There are **6** problems and **7** pages.
- Be sure to write your alias at the top of every page.
- Number each page with the problem number, and page number of your solution (e.g. “Problem 3, p. 1/4” is the first page of a four page solution to problem 3).
- **You must show all your work.**

Possibly useful formulas:

Pauli spin matrices:

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

One-dimensional simple harmonic oscillator operators:

$$X = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger), \quad P = -i\sqrt{\frac{\hbar m\omega}{2}}(a - a^\dagger), \quad [a, a^\dagger] = 1,$$

$$a|n\rangle = \sqrt{n}|n-1\rangle, \quad \text{and} \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle.$$

The Hermite polynomials:

$$H_0(y) = 1, \quad H_1(y) = 2y, \quad H_2(y) = 4y^2 - 2$$

$$H_n(y) = (-1)^n e^{y^2} \frac{\partial^n}{\partial y^n} e^{-y^2}$$

Spherical Harmonics:

$$Y_0^0(\theta, \varphi) = \sqrt{\frac{1}{4\pi}} \quad Y_2^{\pm 2}(\theta, \varphi) = \sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{\pm 2i\varphi}$$

$$Y_1^{\pm 1}(\theta, \varphi) = \mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\varphi} \quad Y_2^{\pm 1}(\theta, \varphi) = \mp \sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{\pm i\varphi}$$

$$Y_1^0(\theta, \varphi) = \sqrt{\frac{3}{4\pi}} \cos \theta \quad Y_2^0(\theta, \varphi) = \sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1)$$

Angular momentum raising and lowering operators:

$$L_{\pm} = L_x \pm i L_y$$

$$L_+ |\ell, m\rangle = \hbar [\ell(\ell+1) - m(m+1)]^{1/2} |\ell, m+1\rangle$$

$$L_- |\ell, m\rangle = \hbar [\ell(\ell+1) - m(m-1)]^{1/2} |\ell, m-1\rangle$$

Gaussian Integral:

$$I_0(\alpha) = \int_{-\infty}^{\infty} e^{-\alpha x^2} dx = (\pi/\alpha)^{1/2}, \quad \alpha > 0$$

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PROBLEM 1: Infinite Square Well

For a particle moving in an infinite square well of width $2a$, the potential energy is

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

Its wave function at time $t = 0$ is

$$\psi(x, 0) = \frac{1}{\sqrt{2}} [u_1(x) + u_2(x)]$$

where $u_1(x)$ and $u_2(x)$ are the normalized ground state and first excited state wave functions respectively and they are orthogonal to each other.

- (a) Determine the energy eigenvalues E_1 and E_2 then find the wave function $\psi(x, t)$ as a function of time. (2 points)
- (b) Find the expectation value of its kinetic energy $\langle T \rangle$ with $\psi(x, t)$. (3 points)
- (c) What is the expectation value of its total energy ($\langle E \rangle$)? Explain the relationship between this result and what you found in Part (b). (2 points)
- (d) Evaluate ΔX in this state with $\psi(x, t)$. (3 points)

PROBLEM 2: The Single-Step Potential

A one-dimensional beam of electrons with kinetic energy $E_0 > 0$ and mass m travels in the positive x -direction and is incident on a step-up potential from the left. The step potential is

$$V(x) = V_0 \Theta(x) = \begin{cases} 0 & \text{for } x < 0, \\ V_0 & \text{for } x \geq 0 \end{cases}$$

where V_0 is a positive constant. The beam may be scattered and/or reflected at the origin.

- (a) If $E_0 < V_0$, sketch the wave function for positive and negative x . You may sketch either the real part of the complex wave function or the probability, but you should label your graph clearly. (*1 points*)
- (b) Solve for the wave function for $x < 0$ and $x > 0$ when $E_0 < V_0$. (*2 points*)
- (c) Given that the flux of the incoming beam is Φ_0 for $x < 0$, solve for the flux past a point x_0 where $x > 0$. Again, in this case $E_0 < V_0$. Do not simply state a result. (*2 points*)
- (d) If $E_0 > V_0$ sketch the wave function for positive and negative x . You may sketch either the real part of the complex wave function or the probability, but you should label your graph clearly. (*1 points*)
- (e) Solve for the wave function for $x < 0$ and $x > 0$ when $E_0 > V_0$. (*2 points*)
- (f) Given that the flux of the incoming beam is Φ_0 for $x < 0$, solve for the flux past a point x_0 where $x > 0$ for this case ($E_0 > V_0$). Do not simply state a result. (*2 points*)

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PROBLEM 3: Angular Momentum Operators

The eigenvector of L^2 and L_z is usually expressed as $|\ell, \ell_z\rangle = |\ell, m\rangle$. This is the ℓ_z basis with

$$L_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

for $\ell = 1$.

- (a) Apply the raising and lowering operators and determine L_y with

$$(L_y)_{mn} = \langle \ell = 1, \ell_z = m | L_y | \ell = 1, \ell_z = n \rangle$$

in the form of a 3×3 matrix. (3 points)

- (b) Find the eigenvalues and normalized eigenvectors of L_y . (3 points)
- (c) If a particle is in the state with $\ell_z = -1$, and L_y is measured, what are the possible outcomes and their probabilities? (3 points)
- (d) Take the state in which $\ell_z = 1$. In this state what is the uncertainty $\Delta L_y = \langle (L_y - \langle L_y \rangle)^2 \rangle^{1/2}$? (1 points)

PROBLEM 4: Isotropic Harmonic Oscillator

The Hamiltonian of a one-dimensional harmonic oscillator is

$$H = \frac{1}{2m}P_x^2 + \frac{1}{2}m\omega_0^2X^2.$$

The harmonic oscillator wave function is often written as

$$\psi_n(\xi) = A_n H_n(\xi) e^{-\frac{1}{2}\xi^2}, \quad n = 0, 1, 2, \dots$$

where A_n = normalization constant, $H_n(\xi)$ is a Hermite polynomial and

$$\xi = \alpha x, \quad \text{with} \quad \alpha = \left(\frac{m\omega}{\hbar} \right)^{1/2}.$$

- (a) What are the energy and the parity of the eigenstate associated with quantum number n ? (2 points)

Let us now consider a 3-dimensional isotropic harmonic oscillator with the following Hamiltonian

$$\begin{aligned} H &= H_x + H_y + H_z \\ &= \frac{1}{2m}(P_x^2 + P_y^2 + P_z^2) + \frac{1}{2}m\omega^2(X^2 + Y^2 + Z^2). \end{aligned}$$

The wave function is given by

$$\Psi_{n_x, n_y, n_z}(x, y, z) = \psi_{n_x}(x)\psi_{n_y}(y)\psi_{n_z}(z).$$

- (b) Find the energy, parity, and degeneracy of the lowest three distinct groups of energy levels. (3 points)
- (c) What is the degeneracy of the energy levels with the same quantum number $n = n_x + n_y + n_z$? (2 points)
- (d) The 3-dimensional harmonic oscillator can also be solved in spherical coordinates. Apply your knowledge of angular dependence for various states to find the angular momentum quantum number (ℓ) for the lowest two energy levels studied in part (b). (3 points)

$$\ell = 0, 1, \dots, n-1$$

P4

a) $E = \hbar\omega(n + \frac{1}{2})$

$$\pi|n\rangle = (-1)^n |n\rangle$$

b) $E_n = \hbar\omega(\underbrace{n_x + n_y + n_z}_n + \frac{3}{2})$

$\pi n_x n_y n_z\rangle = (-1)^{n_x + n_y + n_z} n_x n_y n_z\rangle$	$(\begin{smallmatrix} 2 \\ 0 \end{smallmatrix}) = \frac{2!}{2!} = 1$
$ \Psi_{000}\rangle \rightarrow E: \frac{3\hbar\omega}{2} \quad \pi = 1$	$n=0, D=3, (\begin{smallmatrix} 3 \\ 0 \end{smallmatrix}) = \frac{3!}{2!} = 3$
$ \Psi_{100}\rangle \rightarrow E: \frac{5\hbar\omega}{2} \quad \pi = -1$	$n=1, D=3, (\begin{smallmatrix} 3 \\ 1 \end{smallmatrix}) = \frac{3!}{2!} = 3$
$ \Psi_{110}\rangle \rightarrow E: \frac{7\hbar\omega}{2} \quad \pi = 1$	$n=2, D=3, (\begin{smallmatrix} 3 \\ 2 \end{smallmatrix}) = \frac{3!}{2!} = 3$
$ \Psi_{111}\rangle \rightarrow E: \frac{9\hbar\omega}{2} \quad \pi = -1$	$n=3, D=3, (\begin{smallmatrix} 5 \\ 3 \end{smallmatrix}) = \frac{5!}{3!2!} = 10$

c) $g = \binom{n+3-1}{n} = \binom{n+2}{n}$

d) $l = 0, 1, \dots, n-1$

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F-06**PROBLEM 5: Variational Method**

A particle is subject to the linear potential $V(x) = mgx$ but with an infinite potential barrier at $x = 0$, namely

$$V(x) = \begin{cases} mgx & \text{for } x > 0, \text{ and} \\ \infty & \text{for } x \leq 0. \end{cases}$$

Let us choose

$$\psi_\alpha(x) = xe^{-\alpha x}, \quad \alpha > 0$$

as a trial wave function for the ground state.

- (a) Find $\langle \psi_\alpha | \psi_\alpha \rangle$. (2 points)
- (b) Find the expectation value of the Hamiltonian $\langle H \rangle$. (4 points)
- (c) Determine the best bound on the ground state energy of this system using the variational method and the trial wave function given above. (4 points)

P5

$$V(x) = \begin{cases} mgx & \text{for } x > 0 \\ \infty & \text{for } x \leq 0 \end{cases}$$

$$\psi_\alpha(x) = x e^{-\alpha x}, \quad \alpha > 0$$

$$a) \quad \langle \psi_\alpha | \psi_\alpha \rangle = \int_{-\infty}^{+\infty} \psi_\alpha^*(x) \psi_\alpha(x) dx = \int_{-\infty}^{+\infty} x^2 e^{-2\alpha x} dx$$

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

$$dv = e^{-2\alpha x} dx$$

$$v = -\frac{1}{2\alpha} e^{-2\alpha x}$$

$$= -\frac{x^2 e^{-2\alpha x}}{2\alpha} \Big|_0^{\infty} + \frac{1}{\alpha} \int_0^{\infty} x e^{-2\alpha x} dx$$

$$\int u dv = uv - \int v du$$

$$= -\frac{x e^{-2\alpha x}}{2\alpha^2} \Big|_0^{\infty} + \frac{1}{2\alpha^2} \int_0^{\infty} e^{-2\alpha x} dx$$

$$= +\frac{1}{2\alpha^2} \left[\frac{e^{-2\alpha x}}{-2\alpha} \right]_0^{\infty}$$

$$= \frac{1}{4\alpha^3} [-e^{-2\alpha x}]_0^{\infty} = \frac{1}{4\alpha^3}$$

$$N = \frac{a^{-3/2}}{2}$$

$$N^2 = 2a^{3/2}$$

$$b) \quad \langle V \rangle = \int_0^{\infty} \psi^*(x) mgx \psi(x) dx$$

$$= 4mg\alpha^3 \int_0^{\infty} x^3 e^{-2\alpha x} dx$$

$$= 4mg\alpha^3 \left[\frac{e^{-2\alpha x}}{-2\alpha} \left(x^3 - \frac{3x^2}{-2\alpha} + \frac{3 \cdot 2 \cdot x}{(-2\alpha)^2} - \frac{3 \cdot 2 \cdot 1}{(-2\alpha)^3} \right) \right]_0^{\infty}$$

$$= 4mg\alpha^3 \left[\frac{6^3}{2^4 \alpha^4} \right]$$

$$= \frac{3mg}{2\alpha}$$

$$\langle T \rangle = -\frac{\hbar^2}{2m} 4\alpha^3 \int_0^{\infty} \psi^*(x) \frac{d^2}{dx^2} \psi(x) dx$$

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

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

$$= -2\alpha \beta \int_0^{\infty} x e^{-2\alpha x} + \alpha^2 \beta \int_0^{\infty} x^2 e^{-2\alpha x} dx$$

$$= -2\alpha\beta \left[\frac{x e^{-2\alpha x}}{-2\alpha} \Big|_0^\infty + \frac{1}{2\alpha} \int_0^\infty e^{-2\alpha x} dx \right] + \alpha^2 \beta \left[\frac{1}{2\alpha} \int_0^\infty e^{-2\alpha x} dx \right]$$

PROBLEM 6: Perturbation Theory

The unperturbed interaction Hamiltonian of an electron with a magnetic dipole moment $\vec{\mu}_s$ in a strong magnetic field $\vec{B}_0 = B_0 \hat{z}$ is

$$H_0 = -\vec{\mu}_s \cdot \vec{B}_0$$

where

$$\vec{\mu}_s = -\frac{g\mu_B}{\hbar} \vec{S} = -\frac{g\mu_B}{2} \vec{\sigma}$$

and

$$\mu_B = \frac{e\hbar}{2mc}.$$

If the electron is in the state with $s_z = \hbar/2$, and we add a small magnetic field $\vec{B}_1 = B_1 \hat{x}$ with $B_1 \ll B_0$, then we can consider the Hamiltonian as

$$\begin{aligned} H &= H_0 + H_1 \\ H_1 &= \frac{g}{2}(\mu_B)(\vec{B}_1 \cdot \vec{\sigma}) \end{aligned}$$

where H_1 is a perturbing potential and $g = 2$ for the electron.

- Find the first order change in the energy. (2 point)
- Find the second order change in the energy. (3 point)
- Find the first order correction to the state vector. (2 point)
- Calculate the exact energies for $H = H_0 + H_1$. Expand the larger energy in powers of B_1/B_0 with $B_1 \ll B_0$. Show that the term proportional to B_1^2 corresponds to the answer derived in (b). (3 point)

N.B. You must solve parts (a) - (c) by applying perturbation theory.

