
Examination paper for FY2045 Quantum Mechanics I

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15:00–19:00

Part I ($\sim 30\%$)

Answer the following questions in Inspira.

Problem 1 Multiple choice problems

Choose only **one** of the options for each problem.

a) In a system consisting of four electrons with spin $\frac{1}{2}$, which option below lists *all* the possible values for the total spin of the system?

- A** 0 and 1
- B** 0 and $\frac{1}{2}$
- C** 1 and 2
- D** $\frac{1}{2}$ 1 and $\frac{3}{2}$
- E** 0, 1 and 2

b) Consider the normalized state vector $|\psi\rangle = \frac{1}{3}[(1 - 2i)|1\rangle + 2i|2\rangle]$, where $|1\rangle$ and $|2\rangle$ are orthonormal basis vectors. What is $\langle\psi|$, the dual vector of $|\psi\rangle$?

- A** $\langle\psi| = \frac{1}{3}[(1 + 2i)\langle 1| + 2i\langle 2|]$
- B** $\langle\psi| = \frac{1}{3}[\langle 1| + \langle 2|]$
- C** $\langle\psi| = \frac{1}{3}[(1 + 2i)\langle 1| - 2i\langle 2|]$
- D** $\langle\psi| = \frac{1}{3}[(1 - 2i)\langle 1| + 2i\langle 2|]$
- E** $\langle\psi| = \frac{1}{3}[(1 + 2i)\langle 1| + 2i\langle 2|]$

c) A particle is in a state described by

$$|\psi\rangle = A[|1\rangle - |2\rangle + \sqrt{3}|3\rangle], \quad (1)$$

where $|n\rangle$ are orthonormal energy eigenstates. What is the normalization constant A when chosen real and positive?

A $A = \frac{1}{\sqrt{5}}$

B $A = 1$

C $A = 5$

D $A = \frac{1}{5}$

E $A = \frac{1}{3}$

d) The energy eigenvalue of the state $|n\rangle$ is

$$E_n = \epsilon n^2. \quad (2)$$

where $n = 1, 2, 3, \dots$. What is the energy expectation value of the state $|\psi\rangle$ in Eq. (1)?

A $\langle E \rangle = 14\epsilon$

B $\langle E \rangle = \frac{14}{25}\epsilon$

C $\langle E \rangle = \frac{14}{5}\epsilon$

D $\langle E \rangle = 32\epsilon$

E $\langle E \rangle = \frac{32}{5}\epsilon$

e) Four identical non-interacting particles are placed in a system with single-particle energy levels E_n in Eq. (2). When measuring the total energy and total spin of the system, you get $E_{\text{tot}} = 7\epsilon$ and $\mathbf{S}_{\text{tot}}^2 = 2\hbar^2$. Which one of the following statements is true?

A The particles have spin $s = 0$

B The particles must be bosons

C The particles must be fermions

D The particles must have spin $s = 1$

E The system is not in the ground state

f) Two non-interacting electrons with spin $\frac{1}{2}$ are placed in a system with single-particle eigenenergies E_n in Eq. (2). What are the three lowest energies of the total system?

A $\epsilon, 4\epsilon, 9\epsilon$

B $2\epsilon, 5\epsilon, 5\epsilon$

C $2\epsilon, 5\epsilon, 8\epsilon$

D $2\epsilon, 2\epsilon, 5\epsilon$

E $5\epsilon, 10\epsilon, 13\epsilon$

g) A rectangular box with dimensions L_x , L_y and L_z contains 5 identical, non-interacting fermions with spin $\frac{1}{2}$. The single-particle eigenenergies are given by

$$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2m} \left[\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right], \quad (3)$$

where $n_x, n_y, n_z = 1, 2, 3, \dots$, and $L_x = L_y = L$ and $L_z = \frac{2}{3}L$. What are the quantum numbers (n_x, n_y, n_z) of the filled single-particle states of the ground state of the system?

- A 5 particles in $(1, 1, 1)$
- B 2 particles in $(1, 1, 1)$; 2 particles in $(2, 1, 1)$ and 1 in $(1, 2, 1)$ or vice versa
- C 1 particle in $(1, 1, 1)$; 1 particle in $(2, 1, 1)$, $(1, 2, 1)$ and $(1, 1, 2)$; 1 particle in $(2, 2, 1)$
- D 2 particles in $(1, 1, 1)$; 2 particles in $(1, 1, 2)$; 1 in $(2, 1, 1)$ or $(1, 2, 1)$
- E 2 particles in $(1, 1, 1)$; 3 particles in any combination of states with $n_x + n_y + n_z = 4$

h) A static magnetic field is applied to the system in g), such that the single-particle energies become spin-dependent:

$$E_{n_x n_y n_z, \sigma} = E_{n_x n_y n_z} - H\sigma \quad (4)$$

where $\sigma = +1(-1)$ for spin-up (spin-down) particles. For $|H| > H_c$ the state $(1, 1, 2)$ is occupied in the ground state. What is H_c ?

- A $H_c = 0$
- B $H_c = \frac{29}{4} \frac{\hbar^2 \pi^2}{2mL^2}$
- C $H_c = \frac{3}{8} \frac{\hbar^2 \pi^2}{2mL^2}$
- D $H_c = \frac{15}{8} \frac{\hbar^2 \pi^2}{2mL^2}$
- E $H_c = \frac{3}{2} \frac{\hbar^2 \pi^2}{2mL^2}$

Problem 2 Short answer questions

Give a short answer (maximum 2-3 sentences) to **only two** of the three questions below. If three answers are given, the **first two** will be graded. You may use simple equations in your answers.

- a) Why is the variational method such a useful and powerful tool?
- b) What is the physical interpretation of a Dirac bra-ket $\langle a|b\rangle$?
- c) What is the Fermi energy and Fermi momentum in a free fermion gas?

Part II ($\sim 70\%$)

Write your calculations and answers to the following problems on paper. Clearly mark each page and answer with the problem number.

Problem 3 Spin in a magnetic field

Consider a spin $\frac{1}{2}$ particle in a constant magnetic field $\mathbf{B} = B\hat{e}_z$, described by the Hamiltonian

$$\hat{H} = -\frac{2\mu_B B}{\hbar} \hat{S}_z, \quad (5)$$

where $\hat{S}_z$ is the operator for the z -component of the spin, and μ_B is the Bohr magneton.

a) Solve the time-dependent Schrödinger equation to find the two eigenenergies and eigenstates of the system. You are free to use either abstract spin state vectors or spin spinors. *Hint:* The Pauli matrices are given in the formula sheet.

b) At time $t = 0$, the spin is measured to be in the state

$$|\chi\rangle = \frac{1}{\sqrt{3}}|\uparrow\rangle - \sqrt{\frac{2}{3}}i|\downarrow\rangle \quad \Leftrightarrow \quad \chi = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ -i\sqrt{2} \end{pmatrix}, \quad (6)$$

where $|\uparrow\rangle$ and $|\downarrow\rangle$ are the states with spin up and down with respect to the z direction. Calculate the spin and energy expectation values $\langle \mathbf{S} \rangle$ and $\langle H \rangle$ for this state.

c) What is the spin state at times $t > 0$?

Problem 4 Variational principle

A particle with mass m moves within the one-dimensional potential

$$V(x) = \begin{cases} \gamma x, & \text{for } x \geq 0, \\ \infty, & \text{for } x < 0. \end{cases} \quad (7)$$

a) Use the trial wavefunction

$$\psi(x) = \begin{cases} A x e^{-\alpha x}, & \text{for } x \geq 0, \\ 0, & \text{for } x < 0, \end{cases} \quad (8)$$

to calculate the expectation value of the energy, $\langle H \rangle$. *Hint:* The following integral might be useful:

$$\int_0^\infty x^n e^{-\beta x} dx = \beta^{-n-1} n!. \quad (9)$$

- b) Why is this a good trial function for this system?
- c) Use the variational method to find an upper bound for the ground state energy.

Problem 5 3D isotropic harmonic oscillator

A three-dimensional (3D) isotropic harmonic oscillator is described by the Hamiltonian

$$\hat{H} = \frac{\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2}{2m} + \frac{1}{2}m\omega^2(\hat{x}^2 + \hat{y}^2 + \hat{z}^2), \quad (10)$$

where m is the mass of the particle, and $\omega = \sqrt{k/m}$ with spring constant k . The momentum operator $\hat{p}_j$ and position operator $\hat{x}_j$ along direction $j \in \{x, y, z\}$ satisfy the commutation relation $[\hat{x}_j, \hat{p}_j] = i\hbar$, while operators in different directions commute, for instance, $[\hat{p}_x, \hat{y}] = 0$.

- a) The solutions to the Schrödinger equation for a *one-dimensional* harmonic oscillator are

$$\left[\frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \right] |n\rangle = E_n |n\rangle, \quad (11)$$

with eigenenergies $E_n = \hbar\omega \left(n + \frac{1}{2}\right)$ and eigenvectors $|n\rangle$, where $n = 0, 1, 2, \dots$. Show that the 3D harmonic oscillator has eigenenergies

$$E_{n_x n_y n_z} = \hbar\omega \left(n_x + n_y + n_z + \frac{3}{2} \right) \quad (12)$$

and eigenvectors

$$|n_x, n_y, n_z\rangle \equiv |n_x\rangle |n_y\rangle |n_z\rangle. \quad (13)$$

- b) The orbital angular momentum operator is $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$, where $\hat{\mathbf{r}} = (\hat{x}, \hat{y}, \hat{z})$ and $\hat{\mathbf{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$. Show that the Hamiltonian commutes with the z component of the orbital angular momentum, $\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$. Use this to argue/show that the Hamiltonian commutes with all components of $\hat{\mathbf{L}}$ as well as $\hat{\mathbf{L}}^2$.

Hint: The commutation relations in the formula sheet might be useful.

c) The position and momentum operators along direction j can be used to define ladder operators

$$a_j = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x}_j + i \frac{\hat{p}_j}{m\omega} \right), \quad (14)$$

$$a_j^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x}_j - i \frac{\hat{p}_j}{m\omega} \right), \quad (15)$$

which lower or raise the quantum number n_j with 1, respectively. For instance

$$\begin{aligned} a_x |n_x, n_y, n_z\rangle &= \sqrt{n_x} |n_x - 1, n_y, n_z\rangle, \\ a_x^\dagger |n_x, n_y, n_z\rangle &= \sqrt{n_x + 1} |n_x + 1, n_y, n_z\rangle. \end{aligned}$$

Find expressions for the position and momentum operators in terms of the ladder operators, and use them to show that the angular momentum operator $\hat{L}_z$ can be expressed in terms of ladder operators in the following way:

$$\hat{L}_z = i\hbar (a_x a_y^\dagger - a_x^\dagger a_y). \quad (16)$$

d) Find simultaneous eigenstates of $\hat{H}$ and $\hat{L}_z$ with energy $E = \frac{5}{2}\hbar\omega$. What are the angular momentum quantum numbers m of the states?

Hint: It might be useful to remember that a general state with energy E can be expressed as a superposition of states with quantum numbers n_x, n_y, n_z such that $E_{n_x n_y n_z} = E$:

$$|\psi\rangle = \sum_{\{n_x, n_y, n_z | E_{n_x n_y n_z} = E\}} c_{n_x n_y n_z} |n_x, n_y, n_z\rangle.$$

Problem 6 Anisotropic harmonic oscillator

Consider a system described by $H = H_0 + V$, where H_0 is the Hamiltonian in Eq. (10) and

$$\hat{V} = \kappa \hat{z}^2. \quad (17)$$

If κ is sufficiently small, we can use perturbation theory to find the corrections to the energy eigenvalues Eq. (12).

a) Calculate the first order correction to the ground state energy using non-degenerate perturbation theory

$$E^{(1)} = \langle \psi | \hat{V} | \psi \rangle, \quad (18)$$

with $|\psi\rangle = |0, 0, 0\rangle$. *Hint:* Express $\hat{z}$ in terms of the ladder operators $a_z, a_z^\dagger$.

b) For three-fold degenerate bands, the first order corrections are generally given by the equation

$$\det \begin{pmatrix} V_{11} - E^{(1)} & V_{12} & V_{13} \\ V_{21} & V_{22} - E^{(1)} & V_{23} \\ V_{31} & V_{32} & V_{33} - E^{(1)} \end{pmatrix} = 0, \quad (19)$$

with matrix elements $V_{ij} = \langle \psi_i | \hat{V} | \psi_j \rangle$, where $|\psi_j\rangle$, $j = 1, 2, 3$ label the three degenerate states.

Calculate the first order corrections to the first excited states due to the perturbation $\hat{V}$. Is the degeneracy lifted by the perturbation?

c) Show that the exact eigenenergies for $\kappa > -m\omega^2/2$ are

$$E_{n_x n_y n_z} = \hbar\omega (n_x + n_y + 1) + \hbar\omega_z \left(n_z + \frac{1}{2} \right), \quad (20)$$

with $\omega_z = \sqrt{\omega^2 + \frac{2\kappa}{m}}$. Does this agree with what you found using perturbation theory?

A Formula sheet

Schrödinger equation (time-dependent and time-independent)

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle$$
$$\hat{H} |\psi\rangle = E |\psi\rangle$$

Thermodynamics

$$dW = PdV$$

Eigenvalues and eigenvectors

$$\det(A - \lambda I) = 0$$
$$(A - \lambda I)\mathbf{v} = 0$$

Some properties of the Dirac delta function and Heaviside step function

$$\int dx f(x) \delta(x - a) = f(a)$$
$$\frac{1}{2\pi} \int dx e^{i(k-k_0)x} = \delta(k - k_0)$$
$$\Theta(x) = \begin{cases} 1, & x > 0, \\ 0, & x \leq 0. \end{cases}$$
$$\frac{d}{dx} \Theta(x) = \delta(x)$$
$$\int_{-\infty}^{\infty} dx \left[\frac{d}{dx} \delta(x) \right] f(x) = - \int_{-\infty}^{\infty} dx \delta(x) \left[\frac{d}{dx} f(x) \right]$$

Various physical constants

$$\hbar = 1.054\,571\,817 \times 10^{-34} \text{ J s} = 6.582\,119\,569 \times 10^{-16} \text{ eV s}$$
$$m_e = 9.109\,383\,701\,5 \times 10^{-31} \text{ kg}$$
$$e = 1.602\,176\,634 \times 10^{-19} \text{ C}$$
$$c = 299\,792\,458 \text{ m s}^{-1} \approx 3 \times 10^8 \text{ m s}^{-1}$$
$$\mu_0 = \frac{1}{\epsilon_0 c^2} = \frac{4\pi\alpha}{e^2} \frac{\hbar}{c} = 1.256\,637\,062\,12 \times 10^{-6} \text{ N A}^{-2}$$
$$\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c} \approx \frac{1}{137}$$
$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{e^2 m_e} = 5.29 \times 10^{-11} \text{ m}$$

$$\mu_B = \frac{\hbar e}{2m_e} = 9.274\,010\,078\,3 \times 10^{-24} \text{ J T}^{-1} = 5.788\,381\,806\,0 \times 10^{-5} \text{ eV T}^{-1},$$

Commutators and anticommutators

$$\begin{aligned}[A, B] &\equiv AB - BA \\ [AB, C] &= [A, C]B + A[B, C] \\ [A + B, C] &= [A, C] + [B, C] \\ \{A, B\} &\equiv AB + BA \\ [\hat{x}, \hat{p}_x] &= i\hbar \\ [\hat{S}_x, \hat{S}_y] &= i\hbar \hat{S}_z\end{aligned}$$

Pauli matrices

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

Taylor expansion

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d}{dx} \right)^n f(x) \Big|_{x=a} (x-a)^n$$

Some potentially useful integrals

$$\begin{aligned}\int_{-\infty}^{\infty} dx \, e^{-a(x+b)^2} &= \sqrt{\frac{\pi}{a}} \\ \int_{-\infty}^{\infty} dx \, e^{-ax^2+bx+c} &= \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}+c} \\ \int_{-\infty}^{\infty} dx \, x^{2n} e^{-ax^2} &= \left(-\frac{\partial}{\partial a} \right)^n \int_{-\infty}^{\infty} dx \, e^{-ax^2}\end{aligned}$$

Cylindrical coordinates

$$\begin{aligned}x &= r \cos \phi, \quad y = r \sin \phi, \quad z = z \\ \nabla f &= \frac{\partial f}{\partial r} \hat{r} + \frac{1}{r} \frac{\partial f}{\partial \phi} \hat{\phi} + \frac{\partial f}{\partial z} \hat{z} \\ \nabla \cdot \mathbf{A} &= \frac{1}{r} \frac{\partial}{\partial r} (r A_r) + \frac{1}{r} \frac{\partial A_\phi}{\partial \phi} + \frac{\partial A_z}{\partial z} \\ \nabla^2 f &= \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial f}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 f}{\partial \phi^2} + \frac{\partial^2 f}{\partial z^2} \\ \int d\mathbf{r} &= \int dz \, d\phi \, dr \, r\end{aligned}$$

Spherical coordinates

$$x = r \sin \theta \cos \phi, \quad y = r \sin \theta \sin \phi, \quad z = r \cos \theta$$

$$\nabla f = \frac{\partial f}{\partial r} \hat{r} + \frac{1}{r} \frac{\partial f}{\partial \theta} \hat{\theta} + \frac{1}{r \sin \theta} \frac{\partial f}{\partial \phi} \hat{\phi}$$

$$\nabla \cdot \mathbf{A} = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 A_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (A_\theta \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial A_\phi}{\partial \phi}$$

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

$$\int d\mathbf{r} = \int d\phi \, d\theta \, dr \, \sin \theta r^2$$