NTNU – Trondheim
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Department of Physics

Examination paper for FY2045 Quantum Mechanics I

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15:00–19:00

Part I $(\sim 30\%)$

Answer the following questions in Inspera.

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

A $\langle\psi| = \frac{1}{3}\left[(1+2i)|1\rangle + 2i|2\rangle\right]$

B $\langle\psi| = \frac{1}{3}\left[\langle 1| + \langle 2|\right]$

C $\langle\psi| = \frac{1}{3}\left[(1+2i)\langle 1| - 2i\langle 2|\right]$

D $\langle\psi| = \frac{1}{3}\left[(1-2i)\langle 1| + 2i\langle 2|\right]$

E $\langle\psi| = \frac{1}{3}\left[(1+2i)\langle 1| + 2i\langle 2|\right]$

c) A particle is in a state described by

$$|\psi\rangle = A\big[|1\rangle - |2\rangle + \sqrt{3}|3\rangle\big], \tag{1}$$

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

$$E_n = \epsilon n^2. \tag{2}$$

where $n = 1, 2, 3, \ldots$. 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 $\mathbf{S}^2_{\text{tot}} = 2\hbar^2$. 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

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

where $n_x, n_y, n_z = 1, 2, 3, \ldots$, 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:

$$E_{n_x n_y n_z, \sigma} = E_{n_x n_y n_x} - H\sigma \tag{4}$$

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

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

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

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

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

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

a) Use the trial wavefunction

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

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

$$\int_0^\infty x^n e^{-\beta x}\, dx = \beta^{-n-1} n!. \tag{9}$$

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

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

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

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

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

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

and eigenvectors

$$|n_x, n_y, n_z\rangle \equiv |n_x\rangle |n_y\rangle |n_z\rangle. \tag{13}$$

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

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

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

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

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

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:

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

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

$$\hat{V} = \kappa \hat{z}^2. \tag{17}$$

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

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

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

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

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

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

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

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

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

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

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

Taylor expansion

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

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

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

Spherical coordinates

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

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

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

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

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