NTNU – Trondheim
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Department of Physics

Examination paper for FY2045 Quantum Mechanics I

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09:00–13:00

Part I (36%)

Answer the following questions in Inspera.

Problem 1 Multiple choice problems, 10×3 points

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

a) Consider a system consisting of three particles, two of them with spin $\frac{1}{2}$ and one with spin 1. Which option below lists *all* the possible values for the total spin of the system?

A -1, 0 and 1

B $\frac{1}{2}$, $\frac{3}{2}$

C 1 and 2

D $\frac{1}{2}$, 1 and $\frac{3}{2}$

E 0, 1 and 2

b) What is the normalized eigenspinor of $S_y = \frac{\hbar}{2}\sigma_y$ corresponding to the eigenvalue $-\frac{\hbar}{2}$?

A $\chi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

B $\chi = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

C $\chi = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ i\end{pmatrix}$

D $\chi = \begin{pmatrix}0\\ 1\end{pmatrix}$

E $\chi = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -i\end{pmatrix}$

c) Consider the normalized state vector

$$|\psi\rangle = A[3i|1\rangle + (1-2i)|2\rangle + |3\rangle],$$

where $|1\rangle$, $|2\rangle$ and $|3\rangle$ are orthonormal basis vectors. What is $\langle\psi|$, the dual vector of $|\psi\rangle$?

A $\langle\psi| = A\big[3i|1\rangle + (1-2i)|2\rangle + |3\rangle\big]$

B $\langle\psi| = A^*\big[(\langle 1| + \langle 2| + \langle 3|\big]$

C $\langle\psi| = A\big[(-3i)\langle 1| - (1-2i)\langle 2| - \langle 3|\big]$

D $\langle\psi| = A^*\big[(-3i)\langle 1| + (1+2i)\langle 2| + \langle 3|\big]$

E $\langle\psi| = A^*\big[(3i)\langle 1| + (1+2i)\langle 2| + \langle 3|\big]$

d) The wavefunction of a system is presented as

$$|\psi\rangle = A[|\psi_1\rangle + 2i|\psi_2\rangle + 2|\psi_3\rangle], \tag{1}$$

where $|\psi_1\rangle$, $|\psi_2\rangle$ and $|\psi_3\rangle$ are orthonormal basis vectors. What is A, that is the normalization constant, when chosen real and positive?

A $A = 1$

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

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

D $A = \frac{1}{9}$

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

e) Consider that the wavefunction in Eq. (1) above is expressed in terms of the eigenstates $|\psi_n\rangle$ of a one-dimensional harmonic oscillator with eigenergies

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \qquad n = 0, 1, 2, 3, ... \tag{2}$$

What is the expectation value for total energy?

A $\langle E\rangle = \frac{1}{2}\hbar\omega$

B $\langle E\rangle = \frac{9}{2}\hbar\omega$

C $\langle E \rangle = \frac{11}{4}\hbar\omega$

D $\langle E \rangle = \frac{11}{6}\hbar\omega$

E $\langle E \rangle = \frac{17}{6}\hbar\omega$

f) The system is initially prepared in the state

$$\Psi(x,t) = C_1\psi_1(x)e^{-iE_1t/\hbar} + C_2\psi_2(x)e^{-iE_2t/\hbar} \tag{3}$$

where $\psi_1(x)$ and $\psi_2(x)$ are orthonormal eigenstates of the system and $C_1 \neq C_2$ (both constants are real). Which one of the following options holds true?

A The probability density oscillates as a function of time before measurement.

B The probability density is 1.

C The probability density is $|\psi_1(x)|^2 + |\psi_2(x)|^2$.

D After measuring E_1, $\Psi(x,t) = \psi_1(x)$.

E The ratio of the probabilities for measuring E_1 or E_2 is C_1/C_2.

g) Suppose a spin-$\frac{1}{2}$ particle in a spin state $\chi = \frac{1}{\sqrt{5}}\begin{pmatrix}1\\2i\end{pmatrix}$. Which one of the following statements holds true? (Hint: 5 of the 6 eigenspinors are listed as options in Problem 1(b).)

A The probability of measuring $\frac{\hbar}{2}$ ("spin up") for S_z is $\frac{2}{5}$.

B The probability of measuring $-\frac{\hbar}{2}$ ("spin down") for S_z is $\frac{3}{5}$.

C The probability of measuring $\frac{\hbar}{2}$ for S_x is $\frac{1}{2}$.

D The probability of measuring $\frac{\hbar}{2}$ for S_y is $\frac{1}{2}$.

E One can only choose to measure S_z.

h) Consider a particle in one dimension represented by the wave function in momentum space

$$\phi(p) = \begin{cases} C, & \text{for } 0 \leq p \leq p_0, \\ 0, & \text{otherwise.} \end{cases} \tag{4}$$

Which one of the following options holds true?

A $C = \frac{1}{\sqrt{p_0}}, \quad \langle p^2 \rangle = \frac{p_0^2}{3}$.

B $C = \frac{1}{p_0}, \quad \langle p^2 \rangle = \frac{p_0^2}{4}$.

C $C = \frac{\sqrt{2}}{p_0}, \quad \langle p^2 \rangle = \frac{p_0^2}{3}$.

D $C = \frac{1}{\sqrt{2p_0}}, \quad \langle p^2 \rangle = \frac{p_0^2}{6}$.

E $C = \frac{\sqrt{3}}{p_0}, \quad \langle p^2 \rangle = \frac{p_0^2}{5}$.

i) The energy levels of a 2D infinite well are

$$E_{n_x,n_y} = \frac{\hbar^2\pi^2}{2mL^2}\left(n_x^2 + n_y^2\right) = \epsilon\left(n_x^2 + n_y^2\right), \tag{5}$$

where L is the width of the square well and n_x and n_y are positive integer values ($n_x, n_y = 1, 2, 3, ...$). The original wave function is composed as

$$\Psi = \frac{1}{\sqrt{2}}\psi_{11} + \frac{1}{\sqrt{5}}(\psi_{12} + i\psi_{21}) + \frac{1}{\sqrt{10}}\psi_{22} \tag{6}$$

in terms of the eigenstates referring to the combinations of the quantum numbers n_x and n_y. Which one of the following option holds true after the measurement?

A Probability for measuring $E = 5\epsilon$ is 0.2.

B For $E = 5\epsilon$, the wave function becomes $\Psi = \frac{1}{\sqrt{2}}(\psi_{12} + i\psi_{21})$.

C For $E = 9\epsilon$, the wave function becomes $\Psi = \psi_{22}$.

D The three lowest possible total energies are $E = 2\epsilon$, $E = 4\epsilon$, and $E = 5\epsilon$.

E It is not possible to measure $E = 5\epsilon$.

j) Five identical spin-$\frac{1}{2}$ fermions are placed in a 3D anisotropic harmonic oscillator potential. The potential is steeper in the y- and z- directions, with the oscillator frequencies $\omega_y = 2\omega$ and $\omega_z = 3\omega$, while $\omega_x = \omega$. The single-particle energy levels are:

$$E_{n_x,n_y,n_z} = \hbar\omega\left(n_x + \frac{1}{2}\right) + 2\hbar\omega\left(n_y + \frac{1}{2}\right) + 3\hbar\omega\left(n_z + \frac{1}{2}\right), \tag{7}$$

where n_x, n_y, and n_z are non-negative integers. What are the total energies corresponding to the three lowest-energy configurations (n_x,n_y,n_z) this system of five fermions can have?

A $15\hbar\omega, 15\hbar\omega, 15\hbar\omega$

B $18\hbar\omega, 20\hbar\omega, 23\hbar\omega$

C $19\hbar\omega, 20\hbar\omega, 20\hbar\omega$

D $19\hbar\omega, 20\hbar\omega, 21\hbar\omega$

E $19\hbar\omega, 21\hbar\omega, 23\hbar\omega$

Problem 2 Short answer questions, 3×2 points

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

a) Are the ladder operators of the one-dimensional harmonic oscillator Hermitian?

b) Is it possible to use the variational method for estimating eigenstate energies above the ground state (excited states)?

c) What is the physical origin of the hyperfine structure in the hydrogen atom?

d) What is a coherent state in the context of a harmonic oscillator?

Part II (64%)

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

Problem 3 Addition of angular momentum, 20 points

Consider two particles, one with spin-$\frac{3}{2}$ and the other with spin-$\frac{1}{2}$, corresponding to states $|\frac{3}{2}, m_1\rangle$ and $|\frac{1}{2}, m_2\rangle$, respectively. We shall next consider their coupled angular momentum states.

a) How many possible angular momentum state configurations there will be after angular momentum addition of the individual spin states of the two particles?

b) Instead of using the quantum numbers m_1, and m_2, we can make a change of basis and label the energy eigenstates by j and m_j. These are denoted by $|j, m_j\rangle$, corresponding to an eigenstate of $\hat{\mathbf{J}}^2$. What are the possible values for j and how many m_j-values there are for each j?

c) Now $\hat{\mathbf{J}} = \hat{\mathbf{J}}_1 + \hat{\mathbf{J}}_2$. Demonstrate the commutation relation for $[J_z, J_{1+}]$ by applying it to the state $|j_1 j_2 m_1 m_2\rangle$ directly.

d) Solve $[J^2, J_{1+}]$ by applying commutation relations (we assume $\hat{\mathbf{J}} = \hat{\mathbf{J}}_1 + \hat{\mathbf{J}}_2$ here as well).

e) Express the state $|jm_j\rangle$ for $j = j_{max}$ and $m_j = j_{max}$ in terms of the old states $|m_1 m_2\rangle$. (We have omitted the quantum numbers $\frac{3}{2}$and $\frac{1}{2}$ for individual spins because they are fixed and repeat on both sides of the equations, i.e. $|m_1 m_2\rangle = |\frac{3}{2}\frac{1}{2} m_1 m_2\rangle$ and so on.)

f) Solve the state $|jm_j\rangle$ for $j = j_{max}$ and $m_j = j_{max} - 1$ in terms of $|m_1 m_2\rangle$ by using ladder operators.

g) Solve the state $|jm_j\rangle$ for $j = j_{max}$ and $m_j = j_{max} - 2$ in terms of $|m_1 m_2\rangle$.

h) Solve the state $|jm_j\rangle$ for $j = j_{max} - 1$ and $m_j = j_{max} - 1$ in terms of $|m_1 m_2\rangle$.

Problem 4 Identical particles - bosons, 20 points

Two identical spin-zero bosons are placed in an infinite square well. They interact weakly with each other, via the potential

$$V(x_1, x_2) = -LV_0\delta(x_1 - x_2), \tag{8}$$

where V_0 is a constant and L is the width of the well. (Hint: You might find something useful in the formula sheet.)

a) First, ignoring the interaction between the particles, find the ground state and the first excited state - both the two-particle wave functions and associated energies.

b) Use the first-order perturbation theory to estimate the effect of the particle-particle interaction on the ground state energy. Provide the energy correction and the corrected ground state energy.

c) Do the same for the first excited state energy. Provide the energy correction and the corrected excited state energy. What is the effect of the perturbation in terms of the energy gap between the ground state and the first excited state?

Problem 5 Variational principle - hydrogen atom, 24 points

Our task is to find the upper bound for the ground state energy of hydrogen atom described by the Hamiltonian

$$H = -\frac{\hbar}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} \tag{9}$$

by using a Gaussian trial wave function

$$\psi(r) = Ae^{-br^2}, \tag{10}$$

where A is a real normalisation constant and $b > 0$ is an adjustable parameter. Let us split the problem in tasks.

a) Normalize the wave function, that is solve A.

b) Calculate the expectation value for the potential energy. (Hint: You may find it convenient to use the original A until the final substitution.)

c) Calculate the expectation value of the kinetic energy.

d) Optimize the total energy to find an upper bound $E_{\min}$ for the ground state energy. Here, you should provide the analytical solution. The numerical value follows in the next point.

e) Calculate the numerical value for $E_{\min}$ in electron volts (eV). Compare with the exact result -13.6 eV. Discuss the "goodness" of the trial function for this system. Consider qualitative arguments in comparison with the analytical solution of hydrogen atom.

A Formula sheet

Schrödinger equation (time-dependent and time-independent)

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

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

$$\hbar = 1.054\,571\,817\times 10^{-34}\,\mathrm{J\,s} = 6.582\,119\,569\times 10^{-16}\,\mathrm{eV\,s}$$
$$m_e = 9.109\,383\,701\,5\times 10^{-31}\,\mathrm{kg}$$
$$e = 1.602\,176\,634\times 10^{-19}\,\mathrm{C}$$
$$c = 299\,792\,458\,\mathrm{m\,s^{-1}} \approx 3\times 10^{8}\,\mathrm{m\,s^{-1}}$$
$$\epsilon_0 = 8.854\,187\,812\,8\times 10^{-12}\,\mathrm{F\,m^{-1}}$$
$$\mu_0 = \frac{1}{\epsilon_0 c^2} = \frac{4\pi\alpha}{e^2}\frac{\hbar}{c} = 1.256\,637\,062\,12\times 10^{-6}\,\mathrm{N\,A^{-2}}$$
$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \approx \frac{1}{137}$$
$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{e^2 m_e} = 5.29\times 10^{-11}\,\mathrm{m}$$
$$\mu_B = \frac{\hbar e}{2m_e} = 9.274\,010\,078\,3\times 10^{-24}\,\mathrm{J\,T^{-1}} = 5.788\,381\,806\,0\times 10^{-5}\,\mathrm{eV\,T^{-1}},$$

Commutators and anticommutators

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

Infinite square well in one dimension

$$
\begin{aligned}
\psi_n(x) &= \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \\
E_n &= \frac{n^2\pi^2\hbar^2}{2mL^2}
\end{aligned}
$$

Hydrogen atom

$$
\begin{aligned}
\psi_{1\mathrm{s}}(r) &= \frac{1}{\sqrt{\pi}a_0^{3/2}}e^{-r/a_0} \\
E_n &= -\frac{13.6}{n^2}\mathrm{eV}
\end{aligned}
$$

Ladder operators

$$
\begin{aligned}
a &= \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\hbar\omega}}\hat{p} \\
a^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}
\end{aligned}
$$

Angular momentum

$$
\begin{aligned}
[\hat{J}_i,\hat{J}_j] &= i\hbar\sum\epsilon_{ijk}\hat{J}_k, \qquad k=\{x,y,x,\} \\
\hat{J}^2|j,m\rangle &= \hbar^2 j(j+1)|j,m\rangle \\
\hat{J}_z|j,m\rangle &= \hbar m|j,m\rangle \\
\hat{J}_\pm &= \hat{J}_x \pm i\hat{J}_y \\
\hat{J}_\pm|j,m\rangle &= \sqrt{(j\mp m)(j\pm m+1)}|j,m\pm 1\rangle
\end{aligned}
$$

Pauli matrices

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

Trigonometric relations

$$\begin{aligned}
\sin^2\theta &= \frac{1}{2} - \frac{1}{2}\cos(2\theta) \\
\sin^3\theta &= \frac{3}{4}\sin\theta - \frac{1}{4}\sin(3\theta) \\
\sin^4\theta &= \frac{3}{8} - \frac{1}{2}\cos(2\theta) + \frac{1}{8}\sin(4\theta) \\
\sin^2\theta_1 \sin^2\theta_2 &= \frac{1}{4}\Big[1 - \cos(2\theta_1) - \cos(2\theta_2) + \cos(2\theta_1 - 2\theta_2)\Big]
\end{aligned}$$

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

$$\begin{aligned}
\int_{-\infty}^{\infty} dx\ e^{-a(x+b)^2} &= \sqrt{\frac{\pi}{a}} \\
\int_{-\infty}^{\infty} dx\ e^{-ax^2+bx+c} &= \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}+c} \\
\int_{-\infty}^{\infty} dx\ x^{2n} e^{-ax^2} &= \left(-\frac{\partial}{\partial a}\right)^n \int_{-\infty}^{\infty} dx\ e^{-ax^2} \\
\int_{0}^{\infty} dx\ x^{m} e^{-ax^2} &= \frac{\Gamma(\frac{m+1}{2})}{2a^{(m+1)/2}}, \quad \Gamma(\tfrac{1}{2}) = \sqrt{\pi}, \quad \Gamma(n+1) = n\Gamma(n) \\
\int_{0}^{\infty} dx\ x^{2n+1} e^{-ax^2} &= \frac{n!}{2a^{n+1}}
\end{aligned}$$

Cylindrical coordinates

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

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

$$\boldsymbol{\nabla} \cdot \mathbf{A} = \frac{1}{r}\frac{\partial}{\partial r}(rA_r) + \frac{1}{r}\frac{\partial A_\phi}{\partial \phi} + \frac{\partial A_z}{\partial z}$$

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

$$\int d\mathbf{r} = \int dz\ d\phi\ dr\ r$$

Spherical coordinates

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

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

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

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

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