NTNU – Trondheim
Norwegian University of
Science and Technology

Department of Physics

# Examination paper for FY2045 Quantum Mechanics I

Lecturer: Henning Goa Hugdal

Saturday December 3, 2022
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)** Consider a system of two non-interacting particles. The first particle is in an eigenstate of its operator for the square of the total angular momentum, $\mathbf{J}_1^2$,

$$\mathbf{J}_1^2|j_1, m_1\rangle = \hbar^2 j_1(j_1+1)|j_1, m_1\rangle,$$

with $j_1 = 5$. The second particle is in an eigenstate of its operator for the square of the total angular momentum, $\mathbf{J}_2^2$,

$$\mathbf{J}_2^2|j_2, m_2\rangle = \hbar^2 j_2(j_2+1)|j_2, m_2\rangle,$$

with $j_2 = 2$. The possible values of the square of the total angular momentum operator of the two-particle system are given by

$$\hbar^2 j(j+1).$$

What are the possible values of $j$?

**A** $j = 0, 1, \dots, 5$
**B** $j = 2, 3, 4, 5$
**C** $j = 3, 4, 5, 6, 7$
**D** $j = -7, -6 \dots, 6, 7$
**E** $j = 0, 1, \dots, 7$

**b)** What is the normalized eigenspinor of $S_x = \frac{\hbar}{2}\sigma_x$ 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** $\chi = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

**c)** Which of the following spin states for a spin $\frac{1}{2}$ particle gives a probability of 0.9 of getting the value $\hbar/2$ when measuring the spin along the $x$ direction?

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

**B** $\chi = \frac{1}{\sqrt{5}} \begin{pmatrix} 2 \\ 1 \end{pmatrix}$

**C** $\chi = \frac{1}{\sqrt{5}} \begin{pmatrix} 2 \\ -i \end{pmatrix}$

**D** $\chi = \frac{1}{\sqrt{10}} \begin{pmatrix} 3 \\ 1 \end{pmatrix}$

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

**d)** At time $t = 0$, a particle with spin $\frac{1}{2}$ is measured to be in the spin state

$$\chi(t=0) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \tag{1}$$

a superposition of the energy eigenstates of the system Hamiltonian,

$$H = \hbar\omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2}$$

What is $\chi(t)$, that is, the spin state of the particle at time $t \geq 0$?

**A** $\chi(t) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

**B** $\chi(t) = \begin{pmatrix} e^{-i\omega t} \\ 0 \end{pmatrix}$

**C** $\chi(t) = \begin{pmatrix} 0 \\ e^{i\omega t} \end{pmatrix}$

**D** $\chi(t) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\omega t} \\ e^{i\omega t} \end{pmatrix}$

**E** $\chi(t) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\omega t} \\ e^{-i\omega t} \end{pmatrix}$

**e)** Again, consider the particle described by the Hamiltonian in Eq. (2), measured to be in the spin state in Eq. (1) at $t = 0$. Assuming no measurements have been made since $t = 0$, which of the following statements is true?

**A** If you measure the spin along $x$, you will always get $S_x = \hbar/2$.
**B** At $t = \frac{\pi}{2\omega}$ you are guaranteed to measure $S_y = -\hbar/2$.
**C** It is always impossible to know the outcome of a measurement of $S_y$.
**D** At $t = \frac{\pi}{2\omega}$ you are guaranteed to measure $S_x = -\hbar/2$.
**E** If you measure the energy of the particle, you lose all information about the spin state of the particle.

**f)** In the general formulation of quantum mechanics, the momentum representation is found by considering eigenstates of the momentum operator $\hat{p}$, defined by

$$\hat{p}|p\rangle = p|p\rangle,$$

where $p$ is an eigenvalue. What is $\langle p_2|\hat{p}|p_1\rangle$?

**A** $p_2\delta(p_2 - p_1)$
**B** $\frac{\hbar}{i}\frac{\partial}{\partial p_1}\delta(p_2 - p_1)$
**C** $\delta(p_2 - p_1)$
**D** $0$
**E** $-\frac{\hbar}{i}\frac{\partial}{\partial x}\delta(p_2 - p_1)$

**g)** A particle is described by a wave-packet

$$\Psi(x, t) = \langle x|\Psi\rangle = \int_{-\infty}^{\infty} \phi(k)e^{i[kx-\omega(k)t]}dk, \tag{3}$$

where $\omega(k) = \hbar k^2/(2m)$, and $m$ is the mass of the particle. The coefficients $\phi(k)$ have a distribution

$$\phi(k) = \sqrt{\frac{1}{2\sigma\pi^{3/2}}}e^{-(k-k_0)^2/(2\sigma^2)}, \tag{4}$$

where the constant $\sigma$ is real and larger than 0. The distribution has a large and narrow peak at $k = k_0$, with a finite width. What is momentum-space wavefunction $\Phi(p, t) = \langle p|\Psi\rangle$ corresponding to the wave-packet in Eqs. (3) and (4)? *The following might be useful:* $\psi_p(x) = \langle x|p\rangle = (2\pi\hbar)^{-1/2}e^{ipx/\hbar}$.

**A** $\Phi(p,t) = \phi(p)$

**B** $\Phi(p,t) = \sqrt{2\pi/\hbar}\,\phi(p/\hbar)e^{-ip^2t/(2m\hbar)}$

**C** $\Phi(p,t) = \phi(p/\hbar)e^{-ip^2t/(2m\hbar)}$

**D** $\Phi(p,t) = \phi(p/\hbar)$

**E** $\Phi(p,t) = \sqrt{2\pi\hbar}\,\phi(p/\hbar)e^{-ip^2t/(2m\hbar)}$

**h)** A particle is in the state

$$|\psi\rangle = \sqrt{\frac{2}{6}}|1\rangle + \sqrt{\frac{4}{6}}|2\rangle,$$

where $|1\rangle$ and $|2\rangle$ are energy eigenstates with energies $E_1 = \hbar\omega$ and $E_2 = 2\hbar\omega$, respectively. What is the expectation value of the energy for the state $|\psi\rangle$?

**A** $\langle E\rangle = \frac{3\hbar\omega}{2}$

**B** $\langle E\rangle = \hbar\omega$

**C** $\langle E\rangle = \frac{4\hbar\omega}{3}$

**D** $\langle E\rangle = 2\hbar\omega$

**E** $\langle E\rangle = \frac{5\hbar\omega}{3}$

**i)** Consider the normalized state vector

$$|\psi\rangle = \frac{1}{\sqrt{6}}\left[(2+i)|1\rangle + i|2\rangle\right],$$

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

**A** $\langle\psi| = \frac{1}{\sqrt{6}}\left[(2+i)|1\rangle + i|2\rangle\right]$

**B** $\langle\psi| = \frac{1}{\sqrt{6}}\left[\langle 1| + \langle 2|\right]$

**C** $\langle\psi| = \frac{1}{\sqrt{6}}\left[(2-i)\langle 1| - i\langle 2|\right]$

**D** $\langle\psi| = \frac{1}{\sqrt{6}}\left[(2+i)\langle 1| + i\langle 2|\right]$

**E** $\langle\psi| = \frac{1}{\sqrt{6}}\left[(2-i)\langle 1| + i\langle 2|\right]$

## Problem 2 Short answer questions

Give a short answer (maximum 2-3 sentences) to **two of the three** questions below. You may use simple equations in your answer.

**a)** What are the main differences between fermions and bosons?

**b)** What is the Pauli exclusion principle, and what is the reason behind it?

**c)** Why do physical observables have to be represented by Hermitian operators?

# 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

Consider a three-dimensional box with lengths $L_x = L_y = L$ and $L_z$, where the potential is zero inside and infinite outside.

**a)** Show why the stationary state wavefunctions take the form

$$\psi_{n_x n_y n_z} = A \sin\frac{\pi x n_x}{L} \sin\frac{\pi y n_y}{L} \sin\frac{\pi z n_z}{L_z},\ (0 < x < L,\ 0 < y < L,\ 0 < z < L_z), \tag{5}$$

where $n_x, n_y, n_z$ are positive integers, and that the one-particle energies are given by

$$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2m}\left(\frac{n_x^2 + n_y^2}{L^2} + \frac{n_z^2}{L_z^2}\right), \tag{6}$$

where $m$ is the mass of the particle in the box.

**b)** We place 22 identical non-interacting fermions with spin 1/2 in the box. With $L_z = 0.1L$, what is the maximal occupied one-particle energy $E_{n_x n_y n_z}$ when the system is in the ground state, that is, the total system energy is as low as possible?

**c)** Calculate $N(E)$, the total number of single-particle states with energy less than $E$ in the macroscopic limit ($L$ large) when all sides of the box are equal, $L_x = L_y = L_z = L$. Use the result to calculate the density of states, $g(E)$.

## Problem 4

Derive the equation

$$\frac{d}{dt}\langle F\rangle = \frac{i}{\hbar}\langle[\hat{H}, \hat{F}]\rangle + \left\langle \frac{\partial \hat{F}}{\partial t}\right\rangle \tag{7}$$

using the general definition of an expectation value in the state $|\psi\rangle$,

$$\langle F\rangle = \langle\psi|\hat{F}|\psi\rangle. \tag{8}$$

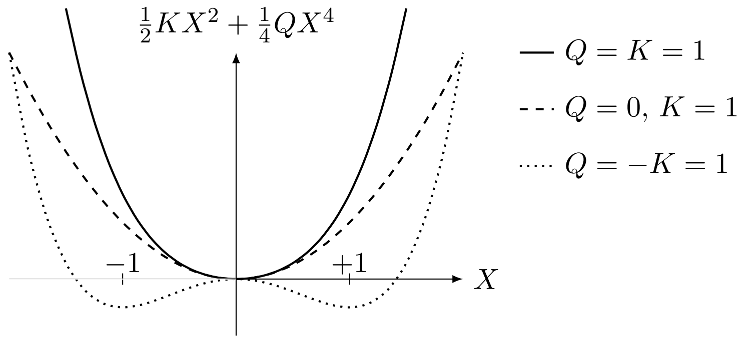
You are free to use any formulation of quantum mechanics. *Hint:* Use the product rule.

## Problem 5

Consider a system described by the Hamiltonian

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}k\hat{x}^2 + \frac{1}{4}q\hat{x}^4, \tag{9}$$

where $k$ and $q$ are real parameters, with $q \geq 0$. A sketch of the potential using dimensionless quantities is shown below.




When $q = 0$ and $k > 0$, Eq. (9) describes a harmonic oscillator, and the Schrödinger equation can be solved by introducing the ladder operators

$$\begin{aligned} a &= \sqrt{\frac{m\omega}{2\hbar}}\left[\hat{x} + \frac{i}{m\omega}\hat{p}_x\right], \\ a^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}\left[\hat{x} - \frac{i}{m\omega}\hat{p}_x\right], \end{aligned} \tag{10}$$

with $\omega \equiv \sqrt{k/m}$. The resulting energies are

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right),\ (n = 0, 1, 2\ldots), \tag{11}$$

with orthonormal eigenstates $|n\rangle$ defined by the eigenvalue equation

$$a^\dagger a|n\rangle = n|n\rangle, \tag{12}$$

and

$$a|0\rangle = 0. \tag{13}$$

**a)** Use Eqs. (10) and (13) to show that the position space wavefunction $\psi_0(x)$ of the ground state of the harmonic oscillator is

$$\psi_0(x) = Ae^{-m\omega x^2/2\hbar}. \tag{14}$$

*Hint:* The following might be useful:

$$\langle x|n\rangle = \psi_n(x),$$
$$1 = \int dx\ |x\rangle\langle x|,$$
$$\langle x''|F(\hat{x},\hat{p}_x)|x'\rangle = F\left(x'', \frac{\hbar}{i}\frac{\partial}{\partial x''}\right)\delta(x''-x').$$

Some of the integration formulas given in the formula sheet might also be useful for this problem.

**b)** Calculate the normalization constant $A$ in Eq. (14).

**c)** We now assume $k > 0$ and $q > 0$ and treat the last term in Eq. (9) as a perturbation, $\hat{V}_q = \frac{1}{4}q\hat{x}^4$. Given the following properties of the raising and lowering operators in Eq. (10),

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

calculate the first-order corrections to the energies using

$$E_n^{(1)} = \langle n|\hat{V}|n\rangle. \tag{17}$$

Briefly comment on the result.

*Hint:* Since the eigenstates $|n\rangle$ are orthonormal, $\langle m|n\rangle = \delta_{nm}$, expectation values containing unequal numbers of raising and lowering operators are zero, e.g. $\langle n|aa^\dagger aa|n\rangle = 0$ etc.

**d)** When $k < 0$ and $q > 0$ we cannot use perturbation theory based on the states $|n\rangle$ and corresponding energies in Eq. (11) — why?

**e)** Calculate the expectation value of the energy, $\langle H\rangle$, when $k < 0$ and $q > 0$ using the trial function

$$\psi_c(x) = Ce^{-m\Omega(x-x_0)^2/2\hbar}, \tag{18}$$

where $\Omega = \sqrt{-2k/m}$ and $x_0$ is a free parameter. *Hint:* It can be useful to shift the integration variables

$$\int_{-\infty}^{\infty} dx\ x^{2n}e^{-a(x-x_0)^2} = \int_{-\infty}^{\infty} dx\ (x+x_0)^{2n}e^{-ax^2}, \tag{19}$$

and keep in mind that $e^{-ax^2}$ is an even function of $x$.

**f)** Use the variational method to find an upper bound for the ground state energy. To simplify the calculations, you can consider the limit $\hbar\Omega q/k^2 \ll 1$ and keep leading order terms in $\hbar\Omega$. Do the results for the upper bound and $x_0$ seem reasonable?

# A Formula sheet

### Schrödinger equation (time-dependent and time-independent)

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

### Thermodynamics

$$dW = PdV$$

### Eigenvalues and eigenvectors

$$\begin{aligned} \det(A - \lambda I) &= 0 \\ (A - \lambda I)\mathbf{v} &= 0 \end{aligned}$$

### Some properties of the Dirac delta function and Heaviside step function

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

### Various physical constants

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

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

**Commutators and anticommutators**

$$\begin{aligned}
[A, B] &\equiv AB - BC \\
[AB, C] &= [A, C]B + A[B, C] \\
[A + B, C] &= [A, C] + [B, C] \\
\{A, B\} &\equiv AB + BA
\end{aligned}$$

**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**

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

**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**

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

**Spherical coordinates**

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

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

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

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

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