# NATIONAL UNIVERSITY OF SINGAPORE

## PC2130 — Quantum Mechanics I

(Semester I: AY 12-13)

Time Allowed: 2 Hours

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### Instructions to candidates

a) This examination paper comprises 10 printed pages, and contains **6** short questions in Part I and **3** longer questions in Part II.

b) Answer **ANY FOUR** (4) questions in Part I. The answers to Part I are to be written on the question paper itself and submitted at the end of the examination.

c) Answer **ALL** the 3 questions in Part II. The answers to Part II are to be written on the answer books.

d) This is a **closed book** examination. Students are allowed to bring in an A4-sized (1 side only) sheet of personal manuscript notes.

e) The total mark for Part I is 20 and that for Part II is 40.

f) No programmable calculators or any other kind of electronic device is allowed during the exam.

g) All answers should be adequately justified.

| Matriculation No. | Marks |
|---|---|
| | |

# Part I – Short Answer Questions

## Problem 1 [5 marks]

If $\hat{Q}$ is an observable that does not depend explicitly on time, and $|u_n\rangle$ is an eigenstate of the Hamiltonian of the system, show that the expectation value of $\hat{Q}$ in the state $|u_n\rangle$ is independent of time.

## Problem 2 [5 marks]

Consider a quantum mechanical system characterized by the Hamiltonian operator $\hat{H}$. Let the normalized state of the system at a given time be represented by the ket $|\psi(t)\rangle$, and consider the *density* operator defined as

$$\hat{\rho}(t) \equiv |\psi(t)\rangle\langle\psi(t)| \,.$$

Show that

$$i\hbar \frac{d}{dt}\hat{\rho}(t) = \left[\hat{H}(t), \hat{\rho}(t)\right] .$$

## Problem 3 [5 marks]

Using the canonical commutation relations between the operators for the position, $\hat{X}$, and momentum, $\hat{P}$:

a) Calculate $\left[\hat{X}, \hat{T}_a\right]$, where $\hat{T}_a = e^{-ia\hat{P}/\hbar}$, and $a \in \mathbb{R}$.

b) Show that $\hat{T}_a \, \hat{X} \, \hat{T}_a^\dagger = \hat{X} - a\hat{\mathbf{1}}$, where $\hat{\mathbf{1}}$ is the identity operator.

## Problem 4 [5 marks]

A particle moving in 1 space dimension is described by the wavefunction

$$\psi(x) = \frac{1}{(x - ic)\,(x + ic)}\, e^{isx}, \qquad (s, c \in \mathbb{R}).$$

a) Calculate the expectation values of the position, $\langle \hat{X} \rangle$, and momentum, $\langle \hat{P} \rangle$.

b) Show that the uncertainty in the momentum in this state cannot be zero.

*Hint: if you find yourself needing to actually evaluate integrals, you are probably not doing it in the most expedient way.*

## Problem 5 [5 marks]

If $|-\rangle_x$ is the eigenstate of the spin projection $\hat{S}_x$ associated with the eigenvalue $-\hbar/2$, calculate

$$ {}_x\langle -|\, e^{i\frac{\pi}{2\hbar}\hat{S}_y}, $$

and express the resulting bra as a linear combination of ${}_z\langle \pm|$, where $|\pm\rangle_z$ are the eigenstates of $\hat{S}_z$.

*Suggestion: write the matrix representation of this expression, and go from there.*

## Problem 6 [5 marks]

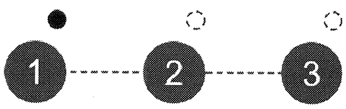
If $|n\rangle$ are the normalized eigenstates of the simple harmonic oscillator, and $\hat{a}$ the annihilation operator, show that the relation $\hat{a}\,|n\rangle = \gamma\,|n-1\rangle$ with $\gamma > 0$ must imply that $\gamma = \sqrt{n}$.

*Suggestion: consider the norm of the kets on both sides of the equation.*

# Part II – Long Answer Questions

## Problem 7 [20 marks]

Consider a simplified model of a triatomic molecule illustrated in the figure below.




One possible basis for the Hilbert space of this system is $\{|x_1\rangle, |x_2\rangle, |x_3\rangle\}$, where each state corresponds to the electron being localized around atom 1, 2, or 3, respectively, and is assumed normalized and orthogonal. In this basis, the Hamiltonian and position operators have the following matrix representation:

$$\hat{H} \longrightarrow \hbar\beta \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix}, \qquad \hat{X} \longrightarrow a \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad (a, \beta > 0)\,.$$

Assume that the system was prepared at $t = 0$ with the electron at atom 1:

$$|\psi(0)\rangle = |x_1\rangle$$

a) What values can a measurement of the energy yield at $t = 0$, and with what probabilities?

b) What is the expectation value, $\langle \hat{H} \rangle$, and the uncertainty, $\delta H = \sqrt{\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2}$, in the energy at $t = 0$?

c) If the system evolves unperturbed from $t = 0$, show that the probability of finding the electron at atom 2 ($x = 0$) at a later time $t$ is

$$p(\mathcal{X} \to 0, t) = \frac{4}{9} \sin^2\left(\frac{3}{2}\beta t\right)$$

d) What is the expectation value, $\langle \hat{H} \rangle$, and the uncertainty, $\delta H = \sqrt{\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2}$, in the energy at time $t$?

e) Are there other times $t > 0$ at which a measurement of the position will reveal the electron at atom 1 again with absolute certainty? If so, when? Justify your answer. *Hint: look at the form of $|\psi(t)\rangle$.*

f) If a measurement of the energy is made at $t = 0$ and one obtains the most likely outcome, what will be the expectation value of the position, $\hat{X}$, immediately after?

## Problem 8 [10 marks]

Consider a particle in the ground state of the following 1D potential

$$V(x) = \begin{cases} 0, & 0 < x < a \\ +\infty, & \text{otherwise} \end{cases}.$$

a) Write the particle's normalized wavefunction and energy.

b) Suddenly, the left wall of the potential is moved to the position $x = -a$, in such a way that the well becomes twice as wide, but the wavefunction of the particle remains unchanged.

   i) Write the solution for all the wavefunctions and energies associated with the eigenstates of the particle in the new potential.
   ii) What is the probability of finding the electron in the ground state of the new potential?
   iii) If the particle's energy is measured, what is the probability of finding an energy that is *not higher* than the one it had before the wall was moved?

*The following identities can be useful:*

$$\sin a \, \sin b = \frac{1}{2} \cos{(a-b)} - \frac{1}{2} \cos{(a+b)}$$

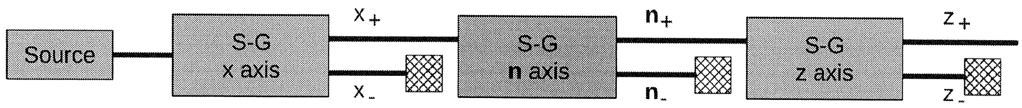
$$\sin a \, \cos b = \frac{1}{2} \sin{(a-b)} + \frac{1}{2} \sin{(a+b)}$$

## Problem 9 [10 marks]

Consider a batch of particles with spin $\frac{1}{2}$. Throughout this problem use the notation $|\pm\rangle_{x,y,z}$ to designate the eigenstates of the spin projections along $x, y, z$, respectively.

a) The particles are initially collimated and prepared in the state $|-\rangle_y$ when they leave the source. Then they go through the Stern-Gerlach selectors shown in the figure below, where the second selector is oriented along the direction of the unit vector $\boldsymbol{n}$:

$$\boldsymbol{n} = \sin\theta\,\boldsymbol{u}_x + \cos\theta\,\boldsymbol{u}_z$$




What (and why) is the fraction of particles coming from the source that leaves the last selector, when

i) $\theta = 0$ ?

ii) $\theta = \pi$ ?

iii) $\theta = \dfrac{\pi}{2}$ ?

b) Imagine that immediately after the last Stern-Gerlach selector discussed in the previous question the collimated beam enters a box of length $L$, inside which there is a constant magnetic field given by

$$\boldsymbol{B} = B\boldsymbol{u}_y \qquad (B > 0)\,.$$

The Hamiltonian that describes the interaction of the magnetic moments with the field is given only by

$$\hat{H} = \omega_0\,\hat{\boldsymbol{S}}\cdot\boldsymbol{u}_y, \qquad \text{where } \omega_0 = \frac{eB}{m},$$

and $\hat{\boldsymbol{S}}$ is the spin operator.

If the atoms travel parallel to the length of the box with a velocity $v_0$, and we want *all* atoms leaving the box to have spin pointing along the positive $\boldsymbol{u}_x$ direction, what size $L$ of the box can make that possible? (express such $L$ in terms of $v_0$ and $\omega_0$).

c) Inside the box containing the constant magnetic field of the previous question, is any of the spin projections $\hat{S}_{x,y,z}$ a constant of the motion? Justify your answer.

...................... **End of Exam Paper** ......................

*VMP*