NATIONAL UNIVERSITY OF SINGAPORE

PC2130 Quantum Mechanics I

(Semester II: AY 2017-18)

Time Allowed: 2 Hours

INSTRUCTIONS TO STUDENTS

1. Please write your student number only. Do **not** write your name.
2. This assessment paper contains **5** questions and comprises 6 printed pages.
3. Students are required to answer **all** questions.
4. Students should write the answers for each question on a new page.
5. This is a CLOSED BOOK examination.
6. Students are allowed to bring in **one A4-sized** help sheet.
7. Non-programmable electronic calculators are allowed.

(1) *Operators and commutators* **[12 points]**

a) Show that for any operators $\hat{A}$ and $\hat{B}$:

$$[\hat{A}, \hat{B}^n] = \sum_{s=0}^{n-1} \hat{B}^s [\hat{A}, \hat{B}] \hat{B}^{n-s-1}, \qquad n = integer > 0.$$

[2 points]

b) Assume now that $[\hat{A}, \hat{B}] = z$, where z is a complex number. Show that

$$[\hat{A}, \hat{B}^n] = n\, z\, \hat{B}^{n-1}.$$

[2 points]

c) Consider the parity operator $\hat{\Pi}$ with

$$\hat{\Pi}\psi(x) = \psi(-x).$$

Show that $\hat{\Pi}$ is Hermitian. [2 points]

d) Derive the eigenvalues of $\hat{\Pi}$, employing that $\hat{\Pi}$ is idempotent: $\hat{\Pi}^2 = \mathbb{1}$.

[2 points]

e) Determine the eigenfunctions of $\hat{\Pi}$. [2 points]

f) In one dimension, the Hamiltonian operator for a free particle is

$$\hat{H} = \frac{1}{2m} \hat{p}_x{}^2$$

and hence $[\hat{H}, \hat{\Pi}] = 0$, implying that $\hat{H}, \hat{\Pi}$ share a common set of eigenfunctions.

Determine the common eigenfunctions for $\hat{H}$ and $\hat{\Pi}$. [2 points]

(2) *1-dimensional delta-function potential* **[12 points]**

Consider the 1D-Schrödinger equation with the delta-function potential

$$V(x) = -\alpha\,\delta(x-a),$$

where α is a positive number and the delta function:

$$\delta(x-a) = \begin{cases} \infty, & x = a \\ 0, & x \neq a \end{cases},$$

and

$$\int_{-\infty}^{\infty} \delta(x-a)dx = 1.$$

a) Determine the bound state energy and corresponding wavefunction.

[6 points]

b) Calculate the reflection coefficient of the delta-function potential $V(x)$ for an incoming plane wave travelling from left to right.

[6 points]

(3) *Asymptotic solutions and power series* **[15 points]**

Consider the spherically symmetric potential $V(r)$:

$$V(r) = -2D\left(\frac{a}{r} - \frac{1}{2}\frac{a^2}{r^2}\right), \qquad with\ constants\ D, a > 0.$$

a) Calculate r_0 such that $V(r_0) = 0$ and r_{min} for which $V(r_{min})$ is minimal. [1 point]

b) Sketch $V(r)$ and indicate the coordinates for r_0 and r_{min}. [1 point]

Consider now the time independent Schrödinger equation and introduce the dimensionless variables:

$$x = \frac{r}{a}, \qquad \beta^2 = -\frac{2ma^2E}{\hbar^2}, \qquad \gamma^2 = \frac{2ma^2D}{\hbar^2}, \qquad E < 0$$

c) Show that the radial part $u(r)$ of the wavefunction $\Psi(\mathbf{r}) = \frac{u(r)}{r} Y_l^m(\theta, \phi)$ satisfies the following differential equation: [3 points]

$$\frac{d^2}{dx^2}u(x) + \left[-\beta^2 + \frac{2\gamma^2}{x} - \frac{\gamma^2 + l(l+1)}{x^2}\right]u(x) = 0.$$

d) Find the asymptotic solutions for $u(x)$ in the limit of $x \to \infty$ and $x \to 0$. [3 points]

e) Hence, or otherwise show that we can express $u(x)$ as: [1 point]

$$u(x) = x^\lambda\, e^{-\beta x}\, f(x), \qquad \lambda = \frac{1}{2} + \sqrt{\gamma^2 + \left(l + \frac{1}{2}\right)^2}.$$

f) Derive the differential equation for $f(x)$. [3 points]

g) Write $f(x)$ as a power series:

$$f(x) = \sum_{i=0}^{\infty} b_i x^i$$

and by demanding that the series stops at power *n*, show that the bound state energies are given by:

$$E_{nl} = -\frac{\hbar^2}{2ma^2}\gamma^4\left[n + \frac{1}{2} + \sqrt{\gamma^2 + \left(l + \frac{1}{2}\right)^2}\right]^{-2}, \qquad n = 0,1,2,\ldots$$

[3 points]

Note: This potential models the vibration spectrum of a di-atomic molecule.

(4) *Schrödinger equation in the presence of magnetic field* **[9 points]**

Consider the Schrödinger equation of a free particle with charge q and mass m in the presence of a magnetic field $\boldsymbol{B}$:

$$i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r},t) = \frac{1}{2m}(\hat{\boldsymbol{p}} - q\boldsymbol{A})^2\,\psi(\boldsymbol{r},t).$$

Bold letters indicate vectors in 3D-space.

$\boldsymbol{A} = \boldsymbol{A}(\boldsymbol{r})$ is the vector potential with $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$,

and the canonical momentum $\hat{\boldsymbol{p}} = \frac{\hbar}{i}\boldsymbol{\nabla}$.

We define the probability density

$$\rho(\boldsymbol{r},t) \equiv \psi^*(\boldsymbol{r},t)\,\psi(\boldsymbol{r},t)$$

and the probability current density in the presence of a magnetic field

$$\boldsymbol{j}(\boldsymbol{r},t) = \frac{\hbar}{2mi}\,(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*) - \frac{q}{m}\boldsymbol{A}\rho.$$

a) The Schrödinger equation in a homogeneous magnetic field yields quantized energy levels (Landau levels) similar to the 1D-harmonic oscillator.

In a semi-classical picture, provide a qualitative argument why energy quantization occurs. [3 points]

b) Show that the continuity equation remains unchanged in the presence of a magnetic field:

$$\frac{\partial}{\partial t}\rho(\boldsymbol{r},t) + \boldsymbol{\nabla}\cdot\boldsymbol{j}(\boldsymbol{r},t) = 0.$$

[6 points]

(5) *Spin in arbitrary direction* **[12 points]**

Consider a spin ½ -system.

We prepare the system in the quantum state

$$|X(t)\rangle = \alpha|\uparrow\rangle e^{+i\omega t} + \beta|\downarrow\rangle e^{-i\omega t},$$

where $|\uparrow\rangle, |\downarrow\rangle$ are eigenstates to the spin-operators $\hat{S}^2, \hat{S}_z$,

α and β are constants with $\alpha^2 + \beta^2 = 1$,

and ω the Larmor frequency.

The operators $\hat{S}_x, \hat{S}_y, \hat{S}_z$ are given by the respective Pauli-matrices

$$\hat{S}_i = \frac{\hbar}{2}\sigma_i, \qquad i = x, y, z.$$

a) Calculate the expectation value $\langle X(t)|\hat{S}_z|X(t)\rangle$. [2 points]

b) Calculate the expectation values $\langle X(t)|\hat{S}_x|X(t)\rangle$ and $\langle X(t)|\hat{S}_y|X(t)\rangle$. [4 points]

c) Consider now the direction defined by the unit vector $\boldsymbol{n}$:

$$\boldsymbol{n} = \begin{pmatrix} sin\theta\ cos\phi \\ sin\theta\ sin\phi \\ cos\theta \end{pmatrix}.$$

Calculate the probability to measure the spin-value $+\frac{1}{2}\hbar$ in the direction of $\boldsymbol{n}$.

[6 points]

-- End of paper --

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