NATIONAL UNIVERSITY OF SINGAPORE

PC3130 QUANTUM MECHANICS II

(Semester I: AY 2023-2024)

Time allowed: 120 minutes

INSTRUCTION TO STUDENTS

1. Please write your student number only. **Please do not write your name.**
2. This assessment paper contains **three** questions and comprises **five** printed pages including this one.
3. Students are required to answer all questions.
4. Question 1 and Question 2 each carries 25 points. Question 3 carries 50 points.
5. Answers to the questions are to be written in the answer books. Please start each question on a new page.
6. This is a CLOSED BOOK exam.
7. You are allowed one double-sided A4-sized help-sheet for this exam.
8. No calculators are allowed for this test.

1. *[Total = 25 points]*

(a) A system of two electrons has a total spin given by $\vec{S}$. The eigenstates of $\vec{S}^2$ and S_z are labeled as $\{|s, m_s\rangle\}$. Explain clearly what is *wrong* with the following statements.
(i) If the two electrons are in the triplet state, either both electrons are in the spin up state, or both electrons are in the spin down state.
(ii) If one electron is in the spin up state and the other electron is in the spin down state, the total spin is zero and the two electrons must be in the singlet state.

(b) Let us consider two electrons in the triplet state. Magnetic dipole interactions between the spins of the two electrons can lead to a splitting in the energies of the spin sublevels given by $\{|s, m_s\rangle\}$, even in the absence of a magnetic field. The Hamiltonian for these spin-spin dipole interactions is given by

$$H = D(S_z^2 - \frac{1}{3}\vec{S}^2) + E(S_x^2 - S_y^2).$$

Here, D and E are known as the zero-field splitting parameters. In this question, we will take $E = 0$ and adopt a system of units in which $\hbar = 1$. Using as the basis $\{|s, m_s\rangle, m_s = 1, 0, -1\}$, show that the matrix representation of H, for $E = 0$, is given by

$$H = \begin{pmatrix} \frac{D}{3} & 0 & 0 \\ 0 & -\frac{2}{3}D & 0 \\ 0 & 0 & \frac{D}{3} \end{pmatrix}.$$

(c) Assuming $D > 0$ and $E = 0$, sketch the energy level diagram for the spin sublevels in the triplet state for the Hamiltonian H in (b). Identify clearly the energy eigenvalues and eigenstates in your energy level diagram.

2. *[Total = 25 points]*

(a) Consider a hydrogen atom that is initially in state $|g\rangle$. A pulsed electric field is applied in the x-direction, resulting in a perturbation

$$V(t) = -qE_0 x\delta(t).$$

Using time-dependent perturbation theory, show that the probability of transition from state $|g\rangle$ to an arbitrary state $|e\rangle$ where $e \neq g$ is given approximately by

$$P_{e\leftarrow g} = \frac{|d_{eg}|^2}{\hbar^2} E_0^2,$$

where d_{eg} is the dipole matrix element between states $|g\rangle$ and $|e\rangle$, i.e., $d_{eg} = q\langle e|x|g\rangle$.

(b) Now suppose we ignore the corrections to the hydrogen atom eigenstates due to the fine structure corrections, so that the eigenstates of the hydrogen atom are given by $|nlm\rangle$, where $\vec{L}^2|nlm\rangle = \hbar^2 l(l+1)|nlm\rangle$, $L_z|nlm\rangle = \hbar m|nlm\rangle$ and n is a positive integer. If the state $|g\rangle$ in (a) is the ground state of the hydrogen atom, for what values of n, l and m can there be non-zero transition probabilities $P_{e\leftarrow g}$, where $|e\rangle \equiv |nlm\rangle$? Briefly explain.

3. Please see also the next page. *[Total = 50 points]*

Consider an electron in a 2D harmonic oscillator potential with Hamiltonian

$$H_0 = \frac{p_x^2 + p_y^2}{2m} + \frac{m\omega^2}{2}(x^2 + y^2),$$

The eigenstates of H_0 are denoted as $|n_x, n_y\rangle$ where n_x and n_y are non-negative integers. The corresponding eigenvalues of H_0 are $E_{n_x,n_y} = \hbar\omega(n_x + \frac{1}{2}) + \hbar\omega(n_y + \frac{1}{2})$. We will examine the Zeeman effect, i.e., the response of this system to an external magnetic field.

(a) Consider the application of a magnetic field $\vec{B} = B\vec{e_z}$ where $\vec{e_z}$ is the unit vector in the z-direction. The perturbation arising from the interaction of the electron orbital angular momentum $\vec{L}$ with $\vec{B}$ is given by $U = -\vec{\mu_L} \cdot \vec{B}$, where $\vec{\mu_L} = -\frac{\mu_B}{\hbar}\vec{L}$. Show that

$$U = \frac{\mu_B B}{\hbar}(xp_y - yp_x).$$

(b) Explain clearly why the first order correction to the ground state of H_0 due to the perturbation U is zero.

(c) Show that the first excited state of H_0 has eigenvalue given by $2\hbar\omega$. State the possible values of n_x and n_y for this first excited state.

(d) Using perturbation theory, find the first order corrections to the energy eigenvalue of the first excited state of H_0 due to the perturbation U.

(e) In practice, the application of $\vec{B}$ leads to changes in the ground state energy of H_0 to first order in B, even though the first order correction due to U is zero. Explain why this is so and sketch what you think the energy level diagram will look like for the ground state of H_0, with and without the application of the magnetic field $\vec{B}$.

Hint: It may be helpful to make use of the ladder operators for harmonic oscillators, which we define here as $\hat{a}$, $\hat{a}^\dagger$, $\hat{b}$ and $\hat{b}^\dagger$.

$$\hat{a}|n_x, n_y\rangle = \sqrt{n_x}|n_x - 1, n_y\rangle\,; \qquad \hat{a}^\dagger|n_x, n_y\rangle = \sqrt{n_x + 1}|n_x + 1, n_y\rangle\,;$$

$$\hat{b}|n_x, n_y\rangle = \sqrt{n_y}|n_x, n_y - 1\rangle\,; \qquad \hat{b}^\dagger|n_x, n_y\rangle = \sqrt{n_y + 1}|n_x, n_y + 1\rangle\,;$$

$$x = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^\dagger + \hat{a})\,; \qquad p_x = i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}^\dagger - \hat{a})\,;$$

$$y = \sqrt{\frac{\hbar}{2m\omega}}(\hat{b}^\dagger + \hat{b})\,; \qquad p_y = i\sqrt{\frac{\hbar m\omega}{2}}(\hat{b}^\dagger - \hat{b})\,.$$

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