

NATIONAL UNIVERSITY OF SINGAPORE

PC3130 QUANTUM MECHANICS II

(Semester I: AY 2022-2023)

Time allowed: 2 hours

INSTRUCTION TO STUDENTS

1. Please write your student number only. **Do not write your name.**
2. This assessment paper contains **four** questions and comprises **six** printed pages including this one.
3. Students are required to answer all questions.
4. Answers to the questions are to be written in the answer books. Please start each question on a new page.
5. This is a **CLOSED BOOK** exam.
6. You are allowed one A4-sized cheat sheet for this exam.
7. No calculators are allowed for this test.

1. Addition of angular momentum [*Total = 25 points*]

An electron in a hydrogen atom is in an orbital with $\ell = 3$. The orbital angular momentum L and spin angular momentum S can be summed to give the total angular momentum $J = L + S$. The eigenstates of the J^2 and J_z operators are labeled as $\{|j, m_j\rangle\}$.

- (a) Which of the following values are allowed values of the total angular momentum quantum number j ?

$$j = \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}, 3, \frac{7}{2}, 4$$

- (b) What are the possible outcomes if you measure the observable J^2 ?
- (c) What are the possible outcomes if you measure the observable $\mathbf{L} \cdot \mathbf{S}$?
- (d) Now suppose that, of the allowed values of j that you found in part (a), the electron is in a state of highest j . Suppose also that $m_j = j$. If you measure the observable L_z , what are the possible outcomes and with what probability will they occur?

2. XXZ Hamiltonian dynamics [Total = 25 points]

The XXZ Hamiltonian describes an anisotropic interaction between two spin $\frac{1}{2}$ atoms. The Hamiltonian is given by

$$H_{\text{XXZ}} = \frac{J_x}{2} (\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y) + J_z \sigma_1^z \sigma_2^z, \quad (1)$$

where J_x and J_z are constants, and σ_n^i describes the Pauli matrix for the i th direction acting on the n th atom. Recall that in the $\{|+\rangle, |-\rangle\}$ basis, the Pauli matrices are

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

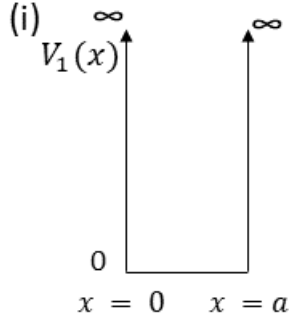
- (a) Calculate the tensor product $\sigma_1^x \sigma_2^x$ as a 4×4 matrix in the $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$ basis.
- (b) Show that the XXZ Hamiltonian from Equation (1) can be written as

$$H_{\text{XXZ}} = \begin{pmatrix} J_z & 0 & 0 & 0 \\ 0 & -J_z & J_x & 0 \\ 0 & J_x & -J_z & 0 \\ 0 & 0 & 0 & J_z \end{pmatrix}.$$

- (c) What is the expectation value $\langle H_{\text{XXZ}} \rangle$ when the system is in the state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$?
- (d) Now suppose each spin $\frac{1}{2}$ atom is allowed to occupy the first two states of a harmonic oscillator, $|\nu=0\rangle$ and $|\nu=1\rangle$. If the two atoms are collectively prepared in the spin state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$, what are the allowed two-atom spatial states in terms of the harmonic oscillator states? Justify your answer.

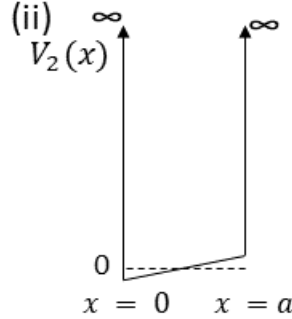
3. Estimating Energy Levels of a Hamiltonian [*Total = 25 points*]

The figure below shows schematics of different potentials in one dimension. We shall, in all cases, consider a single quantum mechanical particle of mass m .



$$V_1(x) = 0 \text{ for } 0 \leq x \leq a$$

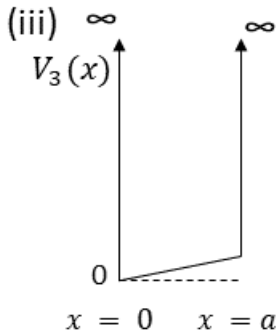
$$V_1(x) \text{ is } \infty \text{ otherwise.}$$



$$V_2(x) = \frac{b}{a} \left(x - \frac{a}{2}\right) \text{ for } 0 \leq x \leq a$$

$$b \ll a$$

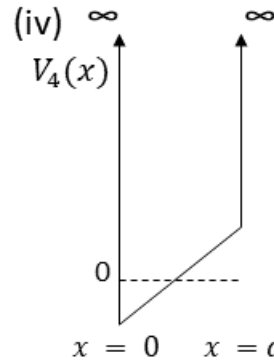
$$V_2(x) \text{ is } \infty \text{ otherwise.}$$



$$V_3(x) = \frac{b}{a} x \text{ for } 0 \leq x \leq a$$

$$b \ll a$$

$$V_3(x) \text{ is } \infty \text{ otherwise.}$$



$$V_4(x) = \frac{b}{a} \left(x - \frac{a}{2}\right) \text{ for } 0 \leq x \leq a$$

$$b \approx a$$

$$V_4(x) \text{ is } \infty \text{ otherwise.}$$

Figure (i) corresponds to the standard (text-book) infinite square well potential. The eigenenergies and eigenstates of the Hamiltonian with potential $V_1(x)$ are given, respectively, by $E_n = \frac{n^2 \hbar^2 \pi^2}{2ma^2}$ and $\psi_n(x) = \sqrt{\frac{2}{a}} \sin(\frac{n\pi x}{a})$, where n is a positive integer.

- (a) Find, correct to first order in $\frac{b}{a}$, the eigenenergies of the Hamiltonian $H = T + V_2$, where T is the kinetic energy operator (refer to Figure (ii) for the form of $V_2(x)$).

- (b) Hence or otherwise, find, correct to first order in $\frac{b}{a}$, the eigenenergies of the Hamiltonian $H = T + V_3$, where T is the kinetic energy operator (refer to Figure (iii) for the form of $V_3(x)$).
- (c) Explain the key difference in approach to estimating the ground state energy of the Hamiltonian with potential V_4 in Figure (iv), compared to estimating the ground state energy of the Hamiltonian with potential given by V_2 or V_3 .
- (d) Let us denote by E_1^* the lowest energy eigenvalue of the Hamiltonian $H = T + V_4$, where T is the kinetic energy operator (refer to Figure (iv) for the form of $V_4(x)$). E_1^* is unknown. Let $E_1 = \frac{\hbar^2 \pi^2}{2ma^2}$.

Only one of the following is strictly correct. Using the variational principle, explain clearly which one of the following is correct:

- (1) $E_1^* > E_1$
- (2) $E_1^* \geq E_1$
- (3) $E_1^* < E_1$
- (4) $E_1^* \leq E_1$
- (5) $E_1^* = E_1$

- (e) Now, using physical intuition, from the form of the potential given in Figure (iv), explain whether or not your answer in (d) makes sense.

4. Time-dependent Perturbation Theory [*Total = 25 points*]

Consider a Hamiltonian $H(t) = H_0 + V(t)$, where H_0 is a time-independent Hamiltonian, and $V(t)$ is a time-dependent perturbation. At time $t = t_0$ before the perturbation is applied, the system is in an initial state $\psi(t_0)$. In the interaction representation, the time-evolution operator satisfies the equation

$$U_I(t, t_0) = 1 + \frac{1}{i\hbar} \int_{t_0}^t V_I(t') U_I(t', t_0) dt'. \quad (2)$$

In this question, you may express your answers entirely in the interaction representation using the subscript I .

- (a) Explain clearly why the interaction representation is useful for the formulation of time-dependent perturbation theory, as opposed to the Schrodinger representation.
- (b) To zeroth order, $U_I(t, t_0) = 1$. By applying $U_I(t, t_0)$ to the initial state $\psi_I(t_0)$ (also in the interaction representation), find the first order correction, $\psi_I^{(1)}(t)$, to the state at time t , due to the perturbation V .
- (c) Using your result in (b), find the first order correction to the expectation value of an operator A at time t due to the perturbation V .
- (d) Derive an expression for the second order correction to the expectation value of A at time t , due to the perturbation V . You may write your final answer in terms of corrections to the state at time t , which you should clearly define.

END OF PAPER [LH QSY]