- You must answer ALL questions in the short answer section.
- You must answer precisely 2 (out of 3) of the questions in the long answer section.

  Please mark clearly which two you have answered below and **start a new sheet for each of the long answer questions**.
- Write your solutions in the indicated space. Scrap paper will not be corrected.
- **You are reminded that Examiners attach great importance to legibility, accuracy and clarity of expression.**
- A simple calculator (without internet access) is allowed.
- Please write your name on the top right corner of each sheet you use.
- Good luck! Enjoy!

NAME STICKER GOES HERE

Short answers: Problem 1	/ 50
Problem A: YES or NO	/ 25
Problem B: YES or NO	/ 25
Problem C: YES or NO	/ 25
Total	/100

Short questions

1. **Quantum States.**

   a) State the three properties an operator ρ must satisfy in order to be a density operator. Deduce from these properties the conditions under which the operator

   $$\rho = \sum_n p_n |\psi_n\rangle\langle\psi_n|$$

   is a density operator, where the set of states $\{|\psi_n\}\}$ are orthonormal.

   (3 marks)

   Properties: $\rho \geq 0, \mathrm{Tr}(\rho) = 1, \rho = \rho^\dagger$ (the last one is automatically fulfilled if its positive).

   Thus we need $p_n > 0 \forall n, \sum_n p_n = 1$.

   b) Explain in terms of a density operator ρ the meaning of the terms *pure state* and *mixed state*. Explain how $\mathrm{Tr}(\rho^2)$ may be used to discriminate between pure and mixed states.

   (3 marks)

   A pure state is a density matrix that has only one non zero eigenvalue. A mixed state can have more than one non-zero eigenvalue. Thus given that $\sum p_n = 1$, $\mathrm{Tr}\,\rho^2 = 1$ iff ρ is pure.

   c) A composite system consisting of components A, B has Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ and its state is

   $$|\psi\rangle = \sum_n \alpha_n |a_n\rangle \otimes |b_n\rangle,$$

   where $\{|a_n\}\}$ and $\{|b_n\}\}$ are orthonormal sets of states. Compute ρ_A, the reduced density operator of system A obtained by tracing over B. Compute ρ_B, defined similarly. Hence show that:

   $$\mathrm{Tr}(\rho_A^2) = \mathrm{Tr}(\rho_B^2)$$

   (4 marks)

   We can easily check that

   $$\mathrm{Tr}_A |\psi\rangle\langle\psi| = \sum \alpha_n^2 \, |a_n\rangle\langle a_n| \tag{1}$$
   $$\mathrm{Tr}_B |\psi\rangle\langle\psi| = \sum \alpha_n^2 \, |b_n\rangle\langle b_n| \tag{2}$$
   $$\tag{3}$$

   Then trivially $\mathrm{Tr}\,\rho_A^2 = \mathrm{Tr}\,\rho_B^2$

2. **Fermions and Bosons.**

a) Explain the difference between Bosonic and Fermionic states.

(3 marks)

Fermionic states have antisymmetric wave-functions, while bosonic ones have symmetric wave-functions (under particle permutation).

b) Consider a three particle state where each particle can be in one of the three states $|a\rangle$, $|b\rangle$, $|c\rangle$. Write down the allowed states of the system if these particles are i. Bosons and ii. Fermions.

(6 marks)

If all the particles are indistinguishable from each other, only symmetric for bosons and anti-symmetric for fermion states will work. This can be readily done by using the Slatter determinant (antisymmetric) and the permanent (symmetric).)

This is the Slatter determinant

$$\psi_{abc}(1,2,3) = \frac{1}{\sqrt{3!}} \begin{vmatrix} \psi_a(1) & \psi_b(1) & \psi_c(1) \\ \psi_a(2) & \psi_b(2) & \psi_c(2) \\ \psi_a(3) & \psi_b(3) & \psi_c(3) \end{vmatrix}$$

And the Permanent

$$\psi_{abc}(1,2,3) = \frac{1}{\sqrt{3!}} \begin{pmatrix} \psi_a(1) & \psi_b(1) & \psi_c(1) \\ \psi_a(2) & \psi_b(2) & \psi_c(2) \\ \psi_a(3) & \psi_b(3) & \psi_c(3) \end{pmatrix} = \psi_a(1)\psi_b(2)\psi_c(3) + \psi_a(1)\psi_b(3)\psi_c(2) + \tag{4}$$

$$+ \psi_a(2)\psi_b(1)\psi_c(3) + \psi_a(2)\psi_b(3)\psi_c(1) + \tag{5}$$

$$+ \psi_a(3)\psi_b(1)\psi_c(2) + \psi_a(3)\psi_b(2)\psi_c(1) \tag{6}$$

Equivalently you can write $\psi_a(x)\psi_b(y)\psi_c(z) = |x, y, z\rangle$. You can look at section 10.3 of the Full Notes for further explanation.

3. **Symmetry**

a) Write down the Cayley table for the permutation group S_3?

(4 marks)

$\circ$	e	(12)	(13)	(23)	(123)	(132)
e	e	(12)	(13)	(23)	(123)	(132)
(12)	(12)	e	(132)	(123)	(13)	(23)
(13)	(13)	(123)	e	(132)	(23)	(12)
(23)	(23)	(132)	(123)	e	(12)	(13)
(123)	(123)	(13)	(23)	(12)	(132)	e
(132)	(132)	(23)	(12)	(13)	e	(123)

b) Describe a physical systems that obeys this symmetry. Write down a representation for the S_3 group that implements the symmetry transformations of this system.

(3 marks)

An equilateral triangle. An example of the representation is the one we have treated in class of the C3v group (see notes/problem sheets) as they are isomorphic.

c) What are the conjugacy classes of S_3? Write down the corresponding character table.

(4 marks)

Equivalently, this are the same as in the C3v group (i.e., see the notes).

4. **Perturbation Theory.**

Consider a Hamiltonian of the form :

$$\hat{H} = \hat{H}_0 + \lambda \hat{V} \tag{7}$$

with :

$$\hat{H}_0 = \epsilon_1 |1\rangle \langle 1| + \epsilon_2 |2\rangle \langle 2| \quad \text{et} \quad \hat{V} = V_{12} |1\rangle \langle 2| + V_{21} |2\rangle \langle 1| \tag{8}$$

where $|1\rangle$ and $|2\rangle$ are the eigenstates of $\hat{H}_0$ associated respectively with the eigenvalues ϵ_1 and ϵ_2. We assume that $\Delta \equiv \epsilon_2 - \epsilon_1 > 0$ and that V_{12} and V_{21} are real.

a) Calculate the exact spectrum of the Hamiltonian as well as its eigenstates.

(5 marks)

The eigenvectors are

$$v_1 = \left(\frac{-\sqrt{4\lambda V_{12}\lambda V_{21} + (\epsilon 1 - \epsilon_2)^2} + \epsilon_1 - \epsilon_2}{\lambda V_{21}\sqrt{\left|\frac{-\epsilon_1+\epsilon_2+\sqrt{(\epsilon_1-\epsilon_2)^2+4\lambda V_{12}\lambda V_{21}}}{\lambda V_{21}}\right|^2 + 4}}, \frac{2}{\sqrt{\left|\frac{-\epsilon_1+\epsilon_2+\sqrt{(\epsilon_1-\epsilon_2)^2+4\lambda V_{12}\lambda V_{21}}}{\lambda V_{21}}\right|^2 + 4}} \right) \tag{9}$$

$$v_2 = \left(\frac{\sqrt{4\lambda V_{12}\lambda V_{21} + (\epsilon_1 - \epsilon_2)^2} + \epsilon_1 - \epsilon_2}{\lambda V_{21}\sqrt{\left|\frac{\epsilon_1-\epsilon_2+\sqrt{(\epsilon_1-\epsilon_2)^2+4\lambda V_{12}\lambda V_{21}}}{\lambda V_{21}}\right|^2 + 4}}, \frac{2}{\sqrt{\left|\frac{\epsilon_1-\epsilon_2+\sqrt{(\epsilon_1-\epsilon_2)^2+4\lambda V_{12}\lambda V_{21}}}{V_{21}}\right|^2 + 4}} \right) \tag{10}$$

b) Using first-order perturbation theory, find the eigenstates and compare with the exact result.

(6 marks)

$$\left|1^{(1)}\right\rangle = |1\rangle + \frac{\lambda V_{12}}{\epsilon_1 - \epsilon_2}|2\rangle \tag{11}$$

$$\left|2^{(1)}\right\rangle = |2\rangle - \frac{V_{21}\lambda}{\epsilon_1 - \epsilon_2}|1\rangle \tag{12}$$

5. **Decoherence.**

Consider a composite system that is prepared in the initial state $|\psi\rangle = \sum_j c_j|E_j\rangle_A \otimes |\phi\rangle_B$ and evolves under a Hamiltonian $H_{AB} = \sum_j |E_j\rangle\langle E_j|_A \otimes H_B^{(j)}$ for time t.

a) Find an expression for the reduced states $\rho_A(t)$ and $\rho_B(t)$ of systems A and B as a function of time.

(4 marks)

$$\rho_B = \sum_j |c_j|^2 e^{-itH_B^{(j)}} |\phi\rangle\langle\phi| e^{itH_B^{(j)}} \tag{13}$$

$$\rho_A = \sum_{j,k} c_j c_k^* |E_j\rangle\langle E_k| \langle\phi| e^{itH_B^{(k)}} e^{-itH_B^{(j)}} |\phi\rangle \tag{14}$$

b) Under what circumstances do A and B remain pure for all times?

(3 marks)

If $H_B^{(j)} = H_B^{(k)} \forall k, j$.

c) Under what circumstances does $\rho_A(t)$ become approximately diagonal in the basis $\{|E_j\rangle\}$?

(2 marks)

If $e^{itH_B^{(j)}}|\phi\rangle = \left|\phi^{(j)}\right\rangle$,then we want to have $\left\langle\phi^{(j)}\middle|\phi^{(k)}\right\rangle = \delta_{j,k}$

Long questions

Please **pick 2 questions** to attempt - mark your choices clearly on the cover sheet.

Start a new sheet for each question.

Question A- Symmetry

1. Prove that the Pauli matrices and the identity (times $\pm 1,\ \pm i$) form a (non-Abelian) group with the matrix product.

   (2 marks)

   Solution:

   A group has to have different properties

   - Closeness: As we know $\sigma_i \sigma_j = i\epsilon_{ijk}\sigma_k$, so the product of two Pauli matrices is a Pauli matrix with a pre-factor of either $\pm 1,\ \pm i$, so the product of each of two possible matrices is in the set of our matrices.
   - Associative: the matrix product is associative.
   - Identity. the group includes the identity matrix.
   - Inverse: $\sigma_i \sigma_i = \mathbb{I}$, $i\sigma_i \times -i\sigma_i = \mathbb{I}$, $-\mathbb{I} \times -\mathbb{I} = \mathbb{I}$. So the inverse of each matrix is in the set of our matrices as well.

2. Prove that if $R(g)$ is a representation of a group G then $R(g) \otimes R(g)$ is also a representation of G.

   (2 marks)

   Solution:

   This can be shown by just seeing that

   $$R(g_1) \otimes R(g_1) \cdot R(g_2) \otimes R(g_2) = R(g_1 g_2) \otimes R(g_1 g_2) \tag{15}$$

3. Consider a unitary irreducible representation $R(g) = U_g$ of group G. Use the Grand Orthogonality Theorem to prove that

   $$\frac{1}{N} \sum_g U_g X U_g^\dagger = \frac{1}{d} \mathrm{Tr}[X]\, I \tag{16}$$

where $d = \dim(X)$ and N is the order of the group.

(4 marks)

Solution:

Because this representation is irreducible, we can use the Grand Orthogonality theorem and rewrite $\frac{1}{N}\sum_g U_g X U_g^\dagger$ as follows.

$$\frac{1}{N}\sum_g U_g X U_g^\dagger = \frac{1}{N}\sum_{jklm}\sum_g [U_g]_{lm} X_{mj} [U_g^\dagger]_{jk} |l\rangle\langle k| \tag{17}$$

$$= \frac{1}{d}\sum_{jklm} \delta_{lk}\delta_{jm} X_{mj} |l\rangle\langle k| \tag{18}$$

$$= \frac{1}{d}\sum_{jk} X_{jj} |k\rangle\langle k| \tag{19}$$

$$= \frac{1}{d}\,\mathrm{Tr}[X] I \tag{20}$$

where $n_a = d$ is the dimension of the vector space of the representation.

4. Use this result to (carefully!) explain why randomly applying either I (i.e, do nothing), σ_x, σ_y, or σ_z (with equal probability) to any single qubit state on average results in the maximally mixed state.

   (3 marks)

   Solution:

   We can consider the group of Pauli matrices and identity with ± 1 and $\pm i$ prefactors that we had in the first part of the question and use the result in the third part to write the average of X.

$$\frac{1}{N}\sum_g U_g \rho U_g^\dagger = \frac{1}{N}\big(4I\rho I + 4\sigma_x\rho\sigma_x + 4\sigma_y\rho\sigma_y + 4\sigma_z\rho\sigma_z\big) \tag{21}$$

$$= \frac{1}{4}\big(I\rho I + \sigma_x\rho\sigma_x + \sigma_y\rho\sigma_y + \sigma_z\rho\sigma_z\big) \tag{22}$$

   where $N = 16$ is the order of the group. So averaging over all elements of the group is equal to randomly applying either I, σ_x, σ_y, or σ_z with probability $\frac{1}{4}$ to any single qubit state. And then from the previous part, we know that it is equal to the maximally mixed state.

$$\frac{1}{4}\big(I\rho I + \sigma_x\rho\sigma_x + \sigma_y\rho\sigma_y + \sigma_z\rho\sigma_z\big) = \frac{1}{2}\mathrm{Tr}[\rho] I = \frac{1}{2} I \tag{23}$$

5. Consider now instead a completely reducible unitary representation $U_g = \oplus_x R_x(g)$ where the $R_x(g)$ are d_x dimensional unitary irreducible representations. It can be shown that

$$\langle X\rangle_G = \frac{1}{N}\sum_g U_g X U_g^\dagger = \frac{1}{d_x}\bigoplus_x \mathrm{Tr}[X\Pi_x]\Pi_x\,. \tag{24}$$

What are Π_x and d_x in this expression?

(3 marks)

Solution: Π_x are the projectors to the irreductible representations and d_x are their dimensions.

6. The above relation for averaging over representations of finite groups, Eq. (24), generalizes to averaging over compact Lie groups. In this case the finite average $\frac{1}{N}\sum_g$ becomes a continuous integral over a uniform measure $\int d\mu(g)$ and we have:

$$\langle X\rangle_G := \int_G d\mu(g) U_g X U_g^\dagger = \frac{1}{d_x}\bigoplus_x \mathrm{Tr}[X\Pi_x]\Pi_x. \tag{25}$$

Use this result to derive an explicit expression (i.e. compute the relevant d_x and Π_x) for the averaged state ρ that results from randomly evolving ρ under the tensor product of two random single qubit unitaries. That is, from apply $U\otimes U$ with $U\in \mathrm{U}(2)$, to any two qubit state ρ, and then averaging:

$$\langle\rho\rangle = \int_{U(2)} d\mu\, U\otimes U\,\rho\, U^\dagger\otimes U^\dagger\ . \tag{26}$$

(5 marks)

Solution:

The easiest way to do this is to find something that commutes with this and that we know how to diagonalise. Then we can use that basis. As we have seen in class $[U\otimes U, \mathrm{SWAP}] = 0$, therefore we can use the SWAP basis to find the projectors of the irreductible representation.

The basis of the $SWAP$ is the symmetric and antisymmetric spaces, i.e. with a eigenvalue $\lambda_+ = 1$

$$|\phi_0\rangle = |00\rangle \tag{27}$$
$$|\phi_1\rangle = |11\rangle \tag{28}$$
$$|\phi_2\rangle = \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle) \tag{29}$$
$$\tag{30}$$

and with eigenvalue $\lambda_- = -1$

$$|\phi_3\rangle = \frac{1}{\sqrt{2}}(|10\rangle - |01\rangle) \tag{31}$$

the corresponding dimensions are $d_+ = 3$, $d_- = 1$. Therefore

$$\frac{1}{3}\mathrm{Tr}\left[\sum_{i=0}^{2}|\phi_i\rangle\langle\phi_i|\,\rho\right]\sum_{i=0}^{2}|\phi_i\rangle\langle\phi_i| \oplus \mathrm{Tr}[|\phi_3\rangle\langle\phi_3|\,\rho]\,|\phi_3\rangle\langle\phi_3| \tag{32}$$

7. Hence (or otherwise) compute the states that result from averaging (i.e, compute $\langle\rho\rangle$ in Eq. (26)) for the following states:

   i. $\rho = |\Phi^+\rangle\langle\Phi^+|$ with $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$

   ii. $\rho = |\Psi^-\rangle\langle\Psi^-|$ with $|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$

   iii. $\rho = |00\rangle\langle 00|$

   iv. An arbitrary tensor product two qubit state $\rho \otimes \sigma$ (hint: use the Bloch vector representation).

   (6 marks)

   Solution:

   i. This state is in the symmetric space, thus

$$\langle\rho\rangle = \frac{1}{3}\left(|\phi_0\rangle\langle\phi_0| + |\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2|\right)$$

   ii. This state is in the anti-symmetric space

$$\langle\rho\rangle = |\phi_3\rangle\langle\phi_3|$$

   iii. This state is in the symmetric space, thus

$$\langle\rho\rangle = \frac{1}{3}\left(|\phi_0\rangle\langle\phi_0| + |\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2|\right)$$

   iv. We denote $\rho = \frac{1}{2}(I + n_x\sigma_x + n_y\sigma_y + n_z\sigma_z)$, $\sigma = \frac{1}{2}(I + m_x\sigma_x + m_y\sigma_y + m_z\sigma_z)$. Then the average state will be

$$\begin{aligned}\langle\rho\otimes\sigma\rangle = &\frac{1}{3}\left(|\phi_0\rangle\langle\phi_0| + |\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2|\right)\frac{1}{4}\left(\sqrt{2}m_x n_x + \sqrt{2}m_y n_y + 2m_z n_z + 2\right)\\ &+ |\phi_3\rangle\langle\phi_3|\,\frac{i(m_y n_x - m_x n_y)}{2\sqrt{2}}\end{aligned}$$

Question B - Variational Principle

Consider the problem of a particle in one dimension, defined by the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \hat{V}(x) \tag{33}$$

The potential $\hat{V}(x)$ takes the form of a well, i.e., $\hat{V}(x) \leq 0 \;\; \forall x$, and $\hat{V}(x) \to 0$ as $|x| \to \infty$. Use the variational principle and the wavefunction ansatz $\psi(x) = A\exp(-\lambda x^2)$, which depends on the variational parameter $\lambda > 0$, to show that there is always at least one bound eigenstate, i.e., with eigenenergy $E_0 < 0$. In particular,

1. State the variational principle and explain how it can be used to estimate the ground state energy of a Hamiltonian H.

   (3 marks)

2. Calculate the normalization factor A.

   (4 marks)

3. Calculate $\langle\psi|\hat{T}(x)|\psi\rangle = \langle\psi|\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)|\psi\rangle$.

   (6 marks)

4. We denote $I(\lambda) = \langle\psi|\hat{V}(x)|\psi\rangle$. So $\langle\psi|\hat{H}|\psi\rangle = \langle\psi|\hat{T}(x)|\psi\rangle + I(\lambda)$. Explicitly write the condition that minimizes the expectation of energy $\langle\psi|\hat{H}|\psi\rangle$. Use the resulting relation to derive an expression for $I(\lambda)$. Use this result in the expression for $\langle\psi|\hat{H}|\psi\rangle$ and demonstrate that we always have $\langle\psi|\hat{H}|\psi\rangle < 0$.

   (9 marks)

5. Explain how the variational principle can be used to find an estimate of the energy of the first excited state of a Hamiltonian. Carefully state any limitations of this approach.

   (3 marks)

You may find the following integrals helpful:

$$\int_{-\infty}^{+\infty} dx \exp\left(-x^2\right) = \sqrt{\pi}$$

$$\int_{-\infty}^{\infty} dx x^2 e^{-\alpha x^2} = \frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}}$$

Question B - Variational Principle: Solution

1. The variational principle consists of the following inequality

$$E_0 \leq \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}, \tag{34}$$

where E_0 is the ground state energy and $|\psi\rangle$ is any wavefunction (in the appropriate Hilbert space).

In practice, one can select a wavefunction ansatz (or trial wavefunction) $\psi(\theta)$, where θ is, in general, a vector of parameters. Though in this problem, we restrict ourselves to a single parameter $\theta = \lambda$. The goal is then to minimize $E(\theta) = \langle\psi(\theta)|H|\psi(\theta)\rangle/\langle\psi(\theta)|\psi(\theta)\rangle$. In the rare cases where $E(\theta)$ can be calculated analytically, it suffices to take the gradient of $E(\theta)$ with respect to θ to find the minima. If instead $E(\theta)$ can only be calculated numerically, the parameters θ can be systematically varied to incrementally lower the energy estimate $E(\theta)$. In both cases, the minimum value of the energy $E(\theta_{\text{min}})$ found will serve as an upper bound on the true ground state energy, that is,

$$E_0 \leq E(\theta_{\text{min}}). \tag{35}$$

2. The normalization factor A is obtained by imposing

$$1 = \int_{-\infty}^{\infty} dx|\psi(x)|^2 = \int_{-\infty}^{\infty} dx|A|^2 e^{-2\lambda x^2} = A^2\sqrt{\frac{\pi}{2\lambda}}, \tag{36}$$

using the known Gaussian integral result. So we find that

$$A = \left(\frac{2\lambda}{\pi}\right)^{1/4}. \tag{37}$$

3. To compute $\langle\psi|T(x)|\psi\rangle$, we will need the second derivative of $\psi(x)$ with respect to x, so we need

$$\frac{d}{dx}e^{-\lambda x^2} = -2\lambda x e^{-\lambda x^2}, \tag{38}$$

$$\frac{d^2}{dx^2}e^{-\lambda x^2} = (-2\lambda + 4\lambda^2 x^2)e^{-\lambda x^2}. \tag{39}$$

To proceed, we simply add a completeness relation, substitute the second derivative result from above, and use the Gaussian integrals provided in the question statement,

$$\langle\psi|T(x)|\psi\rangle = \int_{-\infty}^{\infty} dx\psi^*(x)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\psi(x) \tag{40}$$

$$= -\frac{\hbar^2}{2m}\sqrt{\frac{2\lambda}{\pi}}\int_{-\infty}^{\infty} dx(-2\lambda + 4\lambda^2 x^2)e^{-2\lambda x^2} \tag{41}$$

$$= -\frac{\hbar^2}{2m}\sqrt{\frac{2\lambda}{\pi}}\left(-2\lambda\sqrt{\frac{\pi}{2\lambda}} + 4\lambda^2\frac{1}{4\lambda}\sqrt{\frac{\pi}{2\lambda}}\right) \tag{42}$$

$$= \frac{\lambda\hbar^2}{2m}. \tag{43}$$

4. Now we need to take care of the potential term $I(\lambda) := \langle\psi|V(\hat{x})|\psi\rangle$. Similarly as for the kinetic term, we simply have to add a completeness relation. Here is the calculation one step at a time

$$
\begin{aligned}
I(\lambda) &= \int_{-\infty}^{\infty} dx \langle\psi|V(\hat{x})|x\rangle\langle x|\psi\rangle && (44)\\
&= \int_{-\infty}^{\infty} dx \langle\psi|x\rangle V(x)\langle x|\psi\rangle && (45)\\
&= \int_{-\infty}^{\infty} dx \psi^*(x)V(x)\psi(x) && (46)\\
&= \sqrt{\frac{2\lambda}{\pi}} \int_{-\infty}^{\infty} dx e^{-2\lambda x^2} V(x). && (47)
\end{aligned}
$$

Since we are not provided an explicit form for the potential $V(x)$, we cannot proceed further.

The condition that minimizes the expectation value of the energy is

$$
\min_{\lambda} \langle\psi(\lambda)|H|\psi(\lambda)\rangle = \min_{\lambda} \left(\frac{\lambda\hbar^2}{2m} + \sqrt{\frac{2\lambda}{\pi}} \int_{-\infty}^{\infty} dx e^{-2\lambda x^2} V(x) \right). \tag{48}
$$

By assumption $\lambda > 0$ and $V(x) \leq 0$, so the kinetic expectation value is strictly positive while the potential expectation value is less than or equal to 0.

5. Provided we know the exact form of the ground state, call it $|\psi_0\rangle$, and we take any wavefunction $|\Psi\rangle$ orthogonal to the ground state, that is $\langle\Psi|\psi_0\rangle = 0$, then the following variational principle holds

$$
E_1 \leq \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}, \tag{49}
$$

where E_1 is the energy of the first excited state. The main limitation of this approach is that the ground state should be known. Else we cannot ensure that the wavefunction ansatz we pick is orthogonal to it.

Question C - Entanglement

A quantum system is made of 2 sub-systems and is defined in the Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$, where $\mathcal{H}_1$ and $\mathcal{H}_2$ are the spaces where the 2 sub-systems ares defined. The states of such a system is said to be separable if we can write its density matrix as

$$
\rho_s = \sum_k p_k \rho_k^{(1)} \otimes \rho_k^{(2)}, \tag{50}
$$

with $\sum_k p_k = 1$, $p_k \geq 0$, and $\rho_k^{(1)}$ and $\rho_k^{(2)}$ being density matrices in spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ respectively. A system that cannot be described by a matrix of the form of Eq. (50) is a system with quantum entanglement. (Recall that a density matrix must satisfy the following properties: (i) $\mathrm{Tr}(\rho) = 1$; (ii) $\rho = \rho^\dagger$; (iii) is positive semi-definite.)

1. Show that, for such a separable state, the mean value of an arbitrary observable quantity A_1 of subsystem 1, does not depend on subsystem 2. That is, does not depend on the $\rho_k^{(2)}$.

   (4 marks)

Three players (called Alice, Bob and Charlie) each own a qubit (a quantum system defined in a Hilbert space of dimension 2, with basis $\{|0\rangle, |1\rangle\}$). The three qubit system is in state $|\psi_{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$ (For the rest of the problem, the notation $|ijk\ldots\rangle$, i indicates the qubit state of Alice, j that of Bob, etc.). Alice lives in another galaxy, Bob and Charlie have no knowledge of the total system state.

2. Calculate the mixed state density matrix that describes the subsystem formed by the qubits of Bob and Charlie (In basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$). (2 marks)

3. Show that this matrix is separable. (1 marks)

We now consider the partial transpose operation (not the partial trace). Consider a density matrix ρ describing the state of a system made up of two sub-systems. We indicate with $\{|i\rangle, |j\rangle, \ldots\}$ the states of the basis of the first sub-system; with $\{|\mu\rangle, |\nu\rangle, \ldots\}$ the basis of the second sub-system; and with $\{|i\mu\rangle, |i\nu\rangle, |j\mu\rangle, |j\nu\rangle, \ldots\}$ the total system. If the matrix ρ has elements $\rho_{i\mu,j\nu} = \langle i\mu|\rho|j\nu\rangle$, then the elements of the density matrix ρ^{T_P}, obtained by partial transpose wrt to the subsystem, are defined by $(\rho^{T_P})_{i\mu,j\nu} = \langle i\nu|\rho|j\mu\rangle$.

4. Show that for a separable state of two subsystems, of the form (50), the partial transpose $\rho_s^{T_P}$ with respect to one of the two subsystems is still a valid density matrix. In other words, it still satisfies the three properties (i), (ii), and (iii) mentioned above.

   (4 marks)

5. Hence explain how the partial transpose can be used to determine whether or not a mixed state is entangled.

   (4 marks)

Four actors, named A, B, C, and D (or Alice, Bob, Charlie, and David), each have a quantum bit. The system of the four quantum bits is in the state $|\psi_S\rangle = \frac{1}{2}(|0000\rangle + |0011\rangle + |1100\rangle - |1111\rangle)$. As before, Alice lives in another galaxy. Calculate the density matrix associated with the mixed state that describes the subsystem formed by the quantum bits of Bob, Charlie, and David (in the basis $\{|000\rangle, |001\rangle, |010\rangle, \ldots, |111\rangle\}$).

6. Demonstrate that the mixed state shared by Bob, Charlie, and David is an entangled state. (10 marks)

Question C - Entanglement: Solution

1. Consider operator $A_1 : \hat{H}_1 \mapsto \hat{H}_1$. In the global hilbert space $\hat{H}$, this operator becomes $\hat{A} = \hat{A}_1 \otimes \mathbb{1}_2$. We thus have

$$\begin{aligned}\left\langle \hat{A} \right\rangle &= \mathrm{Tr}\left(\hat{A}_1 \hat{\rho}\right) \\ &= \sum_k p_k \mathrm{Tr}\left(\hat{A}_1 \hat{\rho}_k^{(1)} \otimes \hat{\rho}_k^{(2)}\right) \\ &= \sum_k p_k \mathrm{Tr}\left(\hat{A}_1 \hat{\rho}_k^{(1)}\right) \mathrm{Tr}\left(\hat{\rho}_k^{(2)}\right) \\ &= \sum_k p_k \mathrm{Tr}\left(\hat{A}_1 \hat{\rho}_k^{(1)}\right)\end{aligned}$$

since $\mathrm{Tr}\left(\hat{\rho}_k^{(2)}\right) = 1$ for a density matrix. We have thus shown that $\left\langle \hat{A} \right\rangle$ is independent of $\hat{\rho}_k^{(2)}$

2. The density matrix at pure states $|\psi_{\mathrm{GHZ}}\rangle$ is built as

$$\begin{aligned}\hat{\rho}_0 &= |\psi_{\mathrm{GHZ}}\rangle \langle \psi_{\mathrm{GHZ}}| \\ &= \frac{1}{2}\left(|000\rangle + |111\rangle\right)\left(\langle 000| + \langle 111|\right)\end{aligned}$$

The density matrix for subsystems B and C is given by the partial traces of $\hat{\rho}_0$ on the Alice system

$$\begin{aligned}\hat{\rho} &= \langle 0_A| \hat{\rho}_0 |0_A\rangle + \langle 1_A| \hat{\rho}_0 |1_A\rangle \\ &= \frac{1}{2}\left(|00\rangle \langle 00| + |11\rangle \langle 11|\right) \\ &= \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\end{aligned}$$

3. We note that we can write

$$\hat{\rho} = \frac{1}{2}\left(\hat{\rho}_0^{(1)} \otimes \hat{\rho}_0^{(2)} + \hat{\rho}_1^{(1)} \otimes \hat{\rho}_1^{(2)}\right) \tag{51}$$

where $\hat{\rho}_0^{(j)} = |0\rangle \langle 0|$ and $\hat{\rho}_1^{(j)} = |1\rangle \langle 1|$ are density matrices. By definition, the state is separable.

4. For a separable density matrix $\hat{\rho}_S$, the definition of partial transposition is simply given by
$$\hat{\rho}_S^{T_B} = \sum_k \hat{\rho}_k^{(1)} \otimes \left(\hat{\rho}_k^{(2)}\right)^T \tag{52}$$
but the $(\hat{\rho}_k^{(2)})^T$ are valid density matrices, that is:
$$\begin{aligned} \mathrm{Tr}\left(\hat{\rho}_k^{(2)}\right)^T &= \mathrm{Tr}\left(\hat{\rho}_k^{(2)}\right) = 1 \\ \left(\left(\hat{\rho}_k^{(2)}\right)^T\right)^\dagger &= \left(\hat{\rho}_k^{(2)}\right)^T \\ \left(\hat{\rho}_k^{(2)}\right)^T &\text{ and } \hat{\rho}_k^{(2)} \text{ have the same eigenvalues} \end{aligned}$$
thus $\hat{\rho}_S^{T_B}$ is still a separable density matrix .

5. Using the result from above we can state that if $\hat{\rho}$ is separable, the partial transpose $\hat{\rho}^{T_B}$ is a valid density matrix. In particular, all eigenvalues of $\hat{\rho}^{T_B}$ have to be non-negative. Conversely, if at least one eigenvalue of $\hat{\rho}^{T_B}$ is negative, the state $\hat{\rho}$ must be entangled. This test (called the PPT criterion) is a necessary criterion for any separable state, however it is not sufficient (there are entangled states that also fulfil the criterion).

6. Like before, the pure state of A, B, C and D is described by $\hat{\rho}_0 = |\psi_S\rangle\langle\psi_S|$. We compute the partial trace relative to A
$$\begin{aligned} \hat{\rho} &= \langle 0_A|\hat{\rho}_0|0_A\rangle + \langle 1_A|\hat{\rho}_0|1_A\rangle \\ &= \frac{1}{4}\left(|000\rangle\langle 000| + |000\rangle\langle 011| + |011\rangle\langle 000| + |011\rangle\langle 011|\right) \\ &+\frac{1}{4}\left(|100\rangle\langle 100| - |100\rangle\langle 111| - |111\rangle\langle 100| + |111\rangle\langle 011|\right) \\ &= \frac{1}{4}\begin{pmatrix} 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 \end{pmatrix} \end{aligned}$$
To show that it is a mixed state, we compute the partial transpose relative to C. We see that $\hat{\rho}^{T_C}_{000,011} = \hat{\rho}_{001,010}$ and $\hat{\rho}^{T_C}_{001,010} = \hat{\rho}_{000,011}$ and same for the 2^e diagonal blocks.

Thus

$$\hat{\rho}^{T_C} = \frac{1}{4}\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{53}$$

We can easily calculate the eigenvalues of this block-diagonal structure. For both blocks, the secular equation is $\lambda^2 - 1 = 0$, which gives 2 pairs of eigenvalues $\lambda = \pm 1$. The matrix $\hat{\rho}^{T_C}$ thus has 2 negative eigenvalues, and therefore, it is not a valid density matrix. According to the condition established earlier, we are in a case of a non-separable state and hence, entangled.