PH3102 Quantum Mechanics Assignment 8

Instructor: Dr. Siddhartha Lal Autumn Semester, 2024

Start Date: October 22, 2024 Submission Deadline: October 29, 2024 .

Submit your answers to the Tutor at the start of the tutorial.

Q1. A system of two interacting spins [14 marks]

Consider two quantum spins $\vec{S}_1$ and $\vec{S}_2$ interacting with each other through a Heisenberg-like interaction. The dimensionless Hamiltonian is given by

$$H = J\vec{S}_1 \cdot \vec{S}_2 \ ,$$

where the strength of the interaction is given by the so-called interaction coupling $J > 0$.
(i.) Argue that this Hamiltonian has four eigenstates.

(ii.) In order to find these eigenstates, express the Hamiltonian purely in terms of the total spin $\vec{S}_{\rm tot} = \vec{S}_1 + \vec{S}_2$, $\vec{S}_1$ and $\vec{S}_2$.

(iii.) What are the operators that commute with this Hamiltonian? Use this observation, together with any important spin-commutation relations, to write down *all* the eigenstates of the Hamiltonian as well as their energies.

(iv.) Now focus on the ground state, which is often referred to as a singlet state (why is that?). This state is special because it has spin rotation or SU(2) symmetry, which means that the state is invariant under rotation of the electron's spin. To see this, calculate the total magnetisation of the state in an arbitrary direction $\hat{n} = (n_x, n_y, n_z)$. The operator for this is defined as $\mathcal{S}_{\rm tot}(\hat{n}) = \hat{n} \cdot \vec{S}_{\rm tot}$. Show that the total magnetisation (which is the expectation value of $\mathcal{S}_{\rm tot}(\hat{n})$) in the singlet state is the same irrespective of the direction vector $\hat{n}$. This shows that the singlet state remains unchanged when we rotate our frame of reference.

(v.) Contrast this with the three excited states in the spectrum. How similar or different are they from the singlet state, in terms of SU(2) symmetry? Answer this by computing the total magnetisation along an arbitrary direction $\hat{n}$ in these states as well. Which of these states would describe a "classical" ferromagnet? What class of magnetism would the singlet describe?

Q2. Broken symmetry and a quantum "phase" transition in a toy model [13 marks]

You have already solved above the model of two spin-1/2 moments interacting with each other through an anti-ferromagnetic Heisenberg coupling. Now, by addning a magnetic field that acts on both the spins, we obtain the Hamiltonian

$$H = J\vec{S}_1 \cdot \vec{S}_2 + B\,(S_1^z + S_2^z)\,, \quad J > 0 \ .$$

(i.) This Hamiltonian can again be solved by obtaining the operators that commute with the Hamiltonian. Write down the four eigenstates and their eigenvalues. Plot all of the eigenvalues on the same figure as a function of the magnetic field (consider only $B > 0$).

(ii.) Can you identify the critical value of the magnetic field at which the ground state undergoes a level-crossing of the ground state? What are the ground states on either side of this level-crossing "transition"? The term broken symmetry in the title of the question refers to the fact that during the level crossing, the ground state undergoes a change in one of its symmetries. Which symmetry is that?

(iii.) From your list of eigenstates and eigenvalues, can you guess what happens if you take J to be negative (i.e., ferromagnetic)? What is (are) the ground state(s) in this case? Is there a transition obtained in this case upon tuning the magnetic field?

Q3. A gentle introduction to entanglement: the singlet state [13 marks]

Here, we consider a remarkable property of the singlet state obtained as the ground state of a two spin-1/2 anti-ferromagnetic Heisenberg model: $|\chi\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle \right)$, where the notation $|\uparrow, \downarrow\rangle$ means that the first spin is in its up configuration while the second spin is in its down configuration. Entanglement is defined as the property of a quantum state where the state of a given component depends on the state of another component. Within the singlet state, it can be seen in the fact that measuring one of the spins makes the other spin collapse into the opposite state. In order to make this more concrete, we will calculate the entanglement entropy (EE) of the first spin.

(i.) For this, we must first calculate the density matrix ρ of the state: $\rho = |\chi\rangle \langle\chi|$. The density matrix describes the probabilities of finding a system in various configurations. [To learn more about density matrices, consult Statistical Mechanics by R. K. Pathria, Landau & Lifshitz Statistical Mechanics or Feynman's lectures of Statistical Mechanics.]

(ii.) The next step is to calculate the reduced density matrix ρ_1 for the first spin. This is obtained by taking the density matrix and then tracing over the states of the second spin:

$$\rho_1 = \mathrm{Tr}_2 \left[\rho \right] = \langle \uparrow_2 |\rho| \uparrow_2 | + \langle \downarrow_2 |\rho| \downarrow_2 | \ .$$

(iii.) Following von Neumann, the entanglement entropy (EE) of the first spin is defined as minus of the trace of $\rho_1 \ln \rho_1$. This can be calculated easily by obtaining the eigenvalues $\{\lambda_i\}$ of the matrix ρ_1, and then using the formula $-\mathrm{Tr} \left[\rho_1 \ln \rho_1 \right] = -\sum_i \lambda_i \ln \lambda_i$. The maximum possible EE of a two-component is $\ln 2$. What does this tell you about the singlet state?

(iv.) Intuitively, it is clear that the direct product state $|\uparrow, \downarrow\rangle$ has no entanglement, because measuring one of the spins does not change our knowledge about the other spin. We will now demonstrate this quantitatively. In order to compute the EE of this state and compare it with the singlet, generalise your previous calculation to obtain the EE of the first spin within the state $|\chi(\theta)\rangle = \cos\theta \, |\uparrow, \downarrow\rangle + \sin\theta \, |\downarrow, \uparrow\rangle$. At what value of θ is the EE maximum and when is it minimum? What states do these correspond to?