PH3102: QM Assignment 09

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1 Perturbing the Infinite square well

$\boxed{\textbf{Answer 1.1}}$

There are 2 independent spins $\vec{S}_1$, $\vec{S}_2$ which have two independent Hilbert spaces associated with them. Thus this systems having 2 spins will be described by the tensor product of both Hilbert spaces giving us the labelling $|S_1, m_{S_1}\rangle$ and $|S_2, m_{S_2}\rangle$. Thus to label all the states of the system we need 4 eigenstates.

$\boxed{\textbf{Answer 1.2}}$

The hamiltonian is given as

$$\begin{aligned}
\widehat{H} &= J\hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2 \\
&= \frac{J}{2}\left[\hat{\boldsymbol{S}}_{tot}^2 - \hat{\boldsymbol{S}}_1^2 - \hat{\boldsymbol{S}}_2^2\right]
\end{aligned} \tag{1}$$

Let us write our eigenstates $|S_1, m_{S_1}\rangle \otimes |S_2, m_{S_2}\rangle$ as the tensor product of the eigenstates with the good quantum numbers.

$\boxed{\textbf{Answer 1.3}}$

Since the Spin operators $\hat{\boldsymbol{S}}_1$ and $\hat{\boldsymbol{S}}_2$ acts on independent Hilbert spaces, the operators are independent of each other. We thus have $\left[S_{1i}, S_{2j}\right] = 0$ where $i, j \in \{x, y, z\}$. This gives us the commutation relations $\left[\hat{\boldsymbol{S}}_{tot}, \hat{\boldsymbol{S}}_i\right] = 0, i \in \{1, 2\}$. Thus we see that $\hat{S}_{tot}, \hat{S}_1$ and $\hat{S}_2$ all commute with the Hamiltonian, giving us

$$\left[H, \hat{S}_{tot}\right] = \left[H, \hat{S}_1\right] = \left[H, \hat{S}_2\right] = 0 \tag{2}$$

. We know that we need 4 operators to form a Complete Set of Commuting Observables(CSCO). Let us define $\hat{S}_z = \hat{S}_{1z} + \hat{S}_{2z}$. We know that Spin angular momentum also follows total angular momentum commutation relations. From the addition of angular momenta relations, we get

$$\begin{aligned}
&\left[\hat{\boldsymbol{S}}_{tot}^2, S_z\right] = 0 \\
\Rightarrow &[H, S_z] = 0
\end{aligned} \tag{3}$$

Let us denote our eigenstates as $|\, s, m_s; s_1, s_1\rangle$ where we have

$$\hat{S}_{tot}^2 |s, m_s; s_1, s_2\rangle = s(s+1)\hbar^2 |s, m_s; s_1, s_2\rangle$$

$$\hat{S}_1^2 |s, m_s; s_1, s_2\rangle = s_1(s_1+1)\hbar^2 |s, m_s; s_1, s_2\rangle = \frac{3}{4}\hbar^2 |s, m_s; s_1, s_2\rangle$$

$$\hat{S}_2^2 |s, m_s; s_1, s_2\rangle = s_2(s_2+1)\hbar^2 |s, m_s; s_1, s_2\rangle = \frac{3}{4}\hbar^2 |s, m_s; s_1, s_2\rangle \tag{4}$$

$$S_z |s, m_s; s_1, s_2\rangle = m_s\hbar \ |s, m_s; s_1, s_2\rangle$$

We can then write our reformed hamiltonian as

$$\widehat{H} = \frac{J}{2}\left(\hat{S}_{tot}^2 - \frac{3}{2}\hbar^2 \mathbb{I}\right) \tag{5}$$

We can see that the energy eigenvalue is independent of m_s, thus the levels with same m_s are degenerate. We have already seen before that this is the addition of two spin $1/2$ momenta we thus get the eigenstates

Singlet State

$$|0,0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \quad \left[E_{S=0} = -\frac{3}{4}J\hbar^2\right] \tag{6}$$

Triplet State

$$\left.\begin{array}{l} |1,1\rangle = |\uparrow\uparrow\rangle \\ |1,0\rangle = \frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)] \\ |1,-1\rangle = |\downarrow\downarrow\rangle \end{array}\right\} = \left[E_{S=1} = \frac{1}{4}J\hbar^2\right] \tag{7}$$

Answer 1.4

The operator $\hat{S}_{tot}(\hat{n}) = n_x S_x + n_y S_y + n_z S_z$. Let us now calculate the expectation value of $\hat{S}_{tot}(\hat{n})$ in the ground singlet state.

$$\left\langle \hat{S}_{tot}(\hat{n}) \right\rangle = n_x\langle 0,0|S_x|0,0\rangle + n_y\langle 0,0|S_y|0,0\rangle + n_z\langle 0,0|S_z|0,0\rangle$$

$$= \frac{n_x}{2}\langle 0,0|S_+ + S_-|0,0\rangle + \frac{n_y}{2i}\langle 0,0|S_+ - S_-|0,0\rangle \tag{8}$$

$$= 0$$

We can see that the expectation value is independent of the value of the $\hat{n}$ and thus is exhibits SU(2) symmetry.

Answer 1.5

We now calculate the magnetisations of the three excited states

$$\left\langle \hat{S}_{tot}(\hat{n}) \right\rangle = n_x\langle 1,m|S_x|1,m\rangle + n_y\langle 1,m|S_y|1,m\rangle + n_z\langle 1,m|S_z|1,m\rangle$$

$$= n_z\langle 1,m|S_z|1,m\rangle \tag{9}$$

The total magnetisation for the triplet excited states are

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$$\left\langle \hat{\boldsymbol{S}}_{tot} \right\rangle = \begin{cases} n_z & m = 1 \\ 0 & m = 0 \\ -n_z & m = -1 \end{cases} \tag{10}$$

Classically ferromagnets are magnets with all dipoles aligned in the same direction. Thus the expectation value in the $\hat{z}$ direction is non zero. Thus we have $|1,1\rangle$ and $|1,-1\rangle$ to be classical ferromagnets.

To adequately describe the singlet state we would require another operator called the staggered magnetism operator which gives us anti-ferromagnets. This results in the singlet states being antiferromagnetic.

2 Broken symmetry and a quantum "phase" transition in a toy model

Answer 2.1

We have already calculated for the above Hamiltonian. The new Hamiltonian has a small modification over the previous one. Using Equation 5, The new Hamiltonian simplifies to

$$\begin{aligned}
\widehat{H} &= J\left(\hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2 \right) + B(S_1^z + S_2^z) \\
&= \frac{J}{2}\left(\hat{\boldsymbol{S}}_{tot}^2 - \frac{3}{2}\hbar^2 \mathbb{I} \right) + B S_z
\end{aligned} \tag{11}$$

The eigenstates are the same with different eigenvalues for energy. We can see that the introduction of the magnetic field dependence lifts the degeneracy we saw in the previous step. The Energy eigenvalues are given below

Singlet State $\qquad |0,0\rangle \longrightarrow E_{0,0} = -\frac{3}{4}J\hbar^2$

Triplet States

$$s = 1 : \begin{cases} |1,1\rangle & \longrightarrow E_{1,1} = \frac{1}{4}J\hbar^2 + B\hbar \\ |1,1\rangle & \longrightarrow E_{1,1} = \frac{1}{4}J\hbar^2 \\ |1,-1\rangle & \longrightarrow E_{1,-1} = \frac{1}{4}J\hbar^2 - B\hbar \end{cases} \tag{12}$$
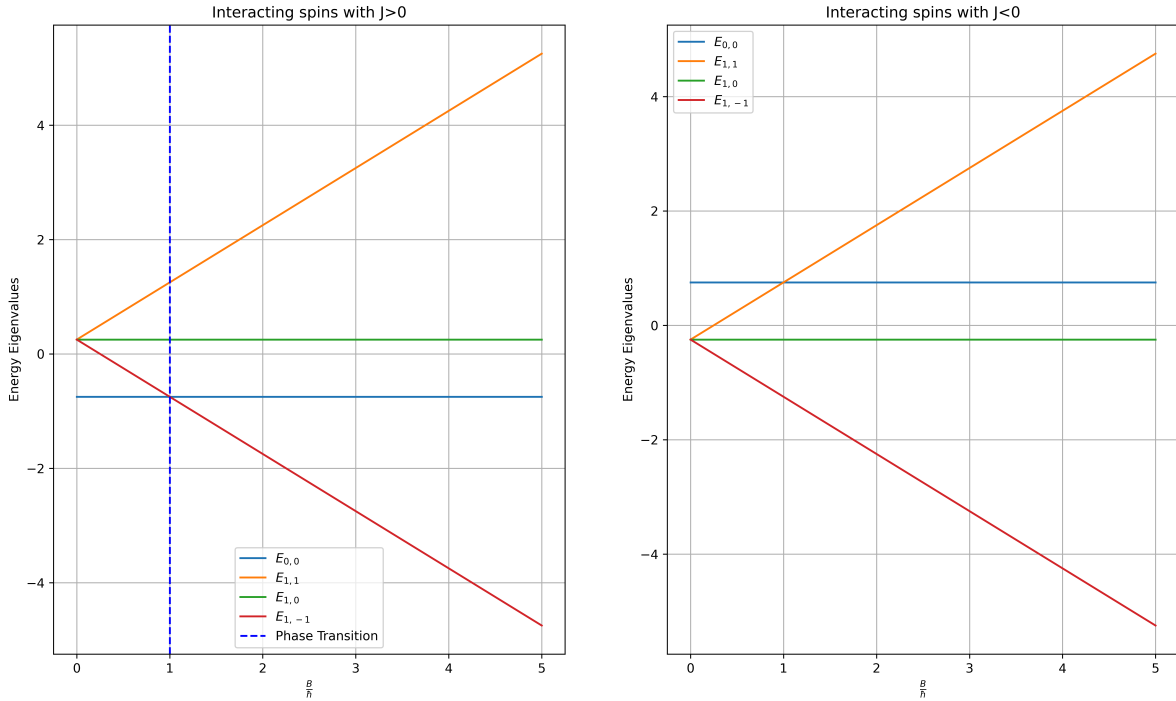
Figure 1: Variation of Energy eigenvalues with $\frac{B}{\hbar}$ for both $J > 0$ and $J < 0$

Answer 2.2

We have $J > 0, B > 0$. From the plot it be can be easily seen that the state $|1, -1\rangle$ crosses the state $|0, 0\rangle$

$$\frac{1}{4}J\hbar^2 - B\hbar = -\frac{3}{4}J\hbar^2 \Rightarrow B = J\hbar \tag{13}$$

Before the crossing the ground state was $|0, 0\rangle$, which after crossing become $|1, -1\rangle$. This causes symmetry breaking. As we saw in Q1 $|0, 0\rangle$ has SU(2) symmetry, but $|1, -1\rangle$ does not have SU(2) symmetry. Thus the ground state no longer has SU(2) symmetry.

Answer 2.3

If we take $J < 0$, as shown in the graph, there is no "phase" transition taking place. $|1, -1\rangle$ is always the ground state. In this case however, the ground state doesnt exhibit SU(2) symmetry.

This can also be expected as again if we consider the staggered magnetism operator, $|0, 0\rangle$ is an antiferromagnetic state. That means that the state has equal spins in opposite directions. However the state $|1, -1\rangle$ is ferromagnetic and has a preferred direction. This causes symmetry breaking.

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3 Gentle introduction to entanglement: the singlet state

Answer 3.1

The singlet state is given as $|\chi\rangle = \frac{1}{2}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$. We will be using the Pauli-Matrix representations. From $\mathbb{H}(2)$, a 2-dimensional hilbert space, the eigenstates of the S_z are represented as

$$|\uparrow\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |\downarrow\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{14}$$

For the two interacting spins, there are two independent 2-dimensional Hilbert spaces, so we know that $|\uparrow\uparrow\rangle = |\uparrow\rangle \otimes |\uparrow\rangle, |\downarrow\downarrow\rangle = |\downarrow\rangle \otimes |\downarrow\rangle |\uparrow\downarrow\rangle = |\uparrow\rangle \otimes |\downarrow\rangle$ and $|\downarrow\uparrow\rangle = |\downarrow\rangle \otimes |\uparrow\rangle$. So we represent all the direct product states

$$|\uparrow\uparrow\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad\qquad |\downarrow\downarrow\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

$$|\uparrow\downarrow\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \qquad\qquad |\downarrow\uparrow\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \tag{15}$$

In the matrix representation , the singlet state is given as

$$|\chi\rangle = \frac{1}{\sqrt{2}} \left\{ \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} - \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \right\} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ -1 \\ 0 \end{bmatrix} \tag{16}$$

The density matrix representation of the singlet state is given as

$$\rho = |\chi\rangle\langle\chi| = \frac{1}{2} \begin{bmatrix} 0 \\ 1 \\ -1 \\ 0 \end{bmatrix} (0, 1, -1, 0) = \frac{1}{2} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{17}$$

Answer 3.2

The density matrix $\rho \in L(\mathbb{H}_1(2) \otimes \mathbb{H}_2(2))$ where $L(\mathbb{H}_1(2) \otimes \mathbb{H}_2(2))$ is the dual of the direct product space. The reduced density matrix elements defined as $\rho_1 \in L(\mathbb{H}_1(2))$ is given as

$$\langle a|\rho_1|b\rangle = \sum_n [\langle a| \otimes \langle n|]\rho[|n\rangle \otimes |b\rangle] \tag{18}$$

where $|a\rangle, |b\rangle$ are the orthonormal eigenkets of $\mathbb{H}_1(2)$ and $|n\rangle$ are the eigenstates of $\mathbb{H}_2(2)$. Thus the matrix elements of ρ_1 are given as

$$\langle\uparrow|\rho_1|\uparrow\rangle = \langle\uparrow\uparrow|\rho|\uparrow\uparrow\rangle + \langle\uparrow\downarrow|\rho|\uparrow\downarrow\rangle = \frac{1}{2} \qquad \langle\uparrow|\rho_1|\downarrow\rangle = \langle\uparrow\uparrow|\rho|\downarrow\uparrow\rangle + \langle\uparrow\downarrow|\rho|\downarrow\downarrow\rangle = 0$$

$$\langle\downarrow|\rho_1|\uparrow\rangle = \langle\downarrow\uparrow|\rho|\uparrow\uparrow\rangle + \langle\downarrow\downarrow|\rho|\uparrow\downarrow\rangle = 0 \qquad \langle\downarrow|\rho_1|\downarrow\rangle = \langle\downarrow\uparrow|\rho|\downarrow\uparrow\rangle + \langle\downarrow\downarrow|\rho|\downarrow\downarrow\rangle = \frac{1}{2}$$

$$(19)$$

The reduced density matrix is

$$\rho_1 = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \frac{1}{2}\mathbb{I} \tag{20}$$

Answer 3.3

The eigenvalues of the reduced density matrix ρ_1 are $\lambda_1 = \lambda_2 = \frac{1}{2}$. Thus the Entanglement Entropy(EE) of the first state

$$S_1 = -\operatorname{Tr}[\rho_1 \ln \rho_1] = -\sum_i \lambda_i \ln \lambda_i = -2\left(\frac{1}{2}\ln\frac{1}{2}\right) = \ln 2 \tag{21}$$

We have that the maximum EE of a two component system is $\ln 2$. This tells us that the singlet spin state is maximally entangled.

Answer 3.4

We want to find the EE of the state $|\chi(\theta)\rangle = \cos(\theta)|\uparrow\downarrow\rangle + \sin(\theta)|\downarrow\uparrow\rangle$ with the first spin state. For this we need to the find the reduced density matrix over the second spin. The density matrix is

$$\rho = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \cos^2\theta & \cos\theta\sin\theta & 0 \\ 0 & \cos\theta\sin\theta & \sin^2\theta & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{22}$$

The reduced density matrix is given by ρ_1

$$\rho_1 = \begin{bmatrix} \cos^2\theta & 0 \\ 0 & \sin^2\theta \end{bmatrix} \tag{23}$$

We want to find the EE of this state. The eigenvalues of ρ_1 are $\lambda_1 = \cos^2\theta, \lambda_2 = \sin^2\theta$. The entanglement Entropy (EE) is given as

$$S_1(\theta) = -\sum_i \lambda_i \ln \lambda_i = -\cos^2\ln(\cos^2\theta) - \sin^2\ln(\sin^2\theta) \tag{24}$$

The graph of $S_1(\theta)$ vs θ to find states of maximal EE is given as
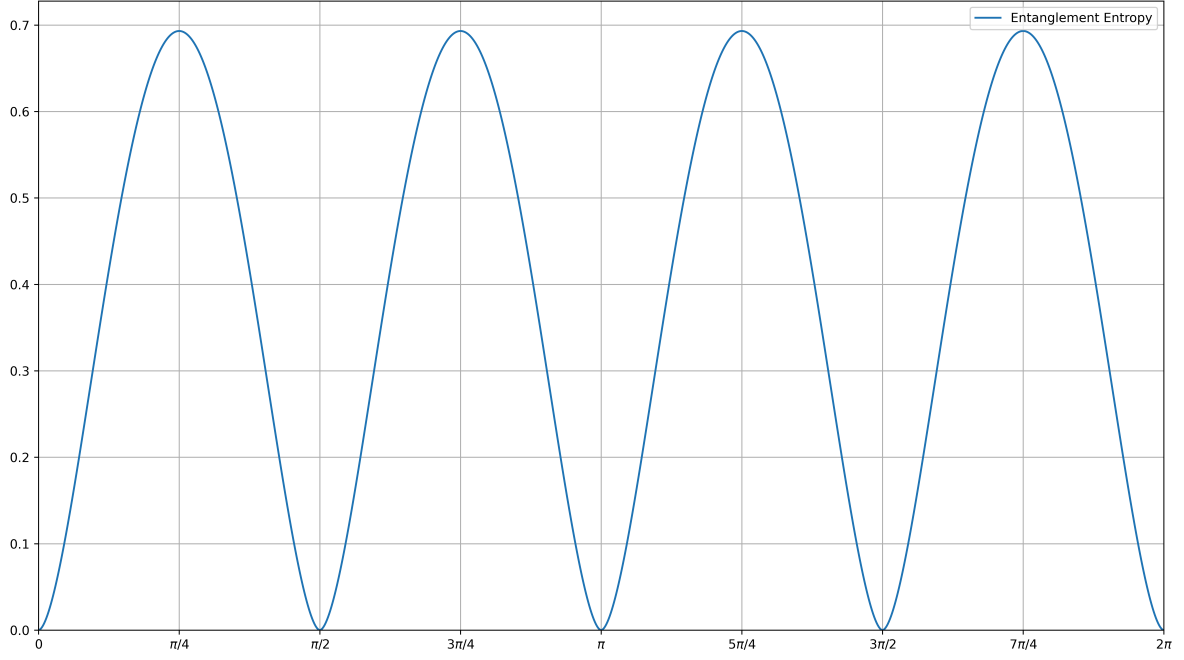
Figure 2: Entanglement Entropy vs θ

The minimal EE is given as $\theta = 0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}$ with $S_1 = 0$ where the corresponding states are not entangled.

The maximal EE is given as $\theta = \frac{\pi}{4}, \frac{3\pi}{4}, \frac{5\pi}{4}, \frac{7\pi}{4}$ with $S_1 = \ln 2$, where the corresponding states are maximally entangled.

The states with minimal and maximal entanglement are

θ	States $S_1(\theta) = 0$
0	$\lvert\uparrow\downarrow\rangle$
$\frac{\pi}{2}$	$\lvert\downarrow\uparrow\rangle$
π	$-\lvert\uparrow\downarrow\rangle$
$\frac{3\pi}{2}$	$-\lvert\uparrow\uparrow\rangle$

θ	States $S_1(\theta) = \ln 2$
$\frac{\pi}{4}$	$\lvert 1, 0\rangle$
$\frac{3\pi}{4}$	$-\lvert 0, 0\rangle$
$\frac{5\pi}{4}$	$-\lvert 1, 0\rangle$
$\frac{7\pi}{4}$	$\lvert 0, 0\rangle$

Table 2: Minimal entanglement states   Table 3: Maximal entanglement states