Solid state systems for quantum information, Session 14

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Exercise 1 : Effective Hamiltonian for the exchange interaction

It is often convenient to work with effective Hamiltonians, which are simpler than the total Hamiltonian of the system, but describe the relevant effects. An example of such an effective Hamiltonian is the exchange interaction term:

$$H_{\text{ex}} = J\vec{s}^{(1)} \cdot \vec{s}^{(2)} = \frac{J}{4}\vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} = \frac{J}{4}(\sigma_x^{(1)}\sigma_x^{(2)} + \sigma_y^{(1)}\sigma_y^{(2)} + \sigma_z^{(1)}\sigma_z^{(2)}). \tag{1}$$

The superscripts in parentheses refer to the first and second particle. The operator $\vec{s}$ is a spin operator (the factor $\hbar$ is omitted for simplicity) and $\vec{\sigma}$ is the vector of Pauli matrices. The quantity J is usually called the "exchange energy".

1. Write H_{ex} in an explicit matrix form, using the basis states $|\uparrow\uparrow\rangle = \left|\uparrow^{(1)}\right\rangle \otimes \left|\uparrow^{(2)}\right\rangle$, $|\uparrow\downarrow\rangle = \left|\uparrow^{(1)}\right\rangle \otimes \left|\downarrow^{(2)}\right\rangle$, $|\downarrow\uparrow\rangle = \left|\downarrow^{(1)}\right\rangle \otimes \left|\uparrow^{(2)}\right\rangle$ and $|\downarrow\downarrow\rangle = \left|\downarrow^{(1)}\right\rangle \otimes \left|\downarrow^{(2)}\right\rangle$ in the order given here.
2. Find the eigenenergies and corresponding eigenstates of H_{ex}. You should find the well-known singlet and the three-degenerate (at zero magnetic field) triplet states.

Exercise 2 : Qubits in double quantum dots: Hund-Mulliken approach

A double quantum dot (DQD) can host two single-spin qubits or, for example, a singlet-triplet qubit. The low-energy spectrum of two electrons in a DQD is often described with a Hund-Mulliken model. Neglecting magnetic field gradients, spin-orbit interaction, and other mechanisms, the Hund-Mulliken approach leads to the simple low-energy Hamiltonian:

$$H = \begin{bmatrix} U+\varepsilon & 0 & -\sqrt{2}t & 0 & 0 & 0 \\ 0 & U-\varepsilon & -\sqrt{2}t & 0 & 0 & 0 \\ -\sqrt{2}t & -\sqrt{2}t & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & g\mu_B B_z & 0 & 0 \\ 0 & 0 & 0 & 0 & -g\mu_B B_z & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{2}$$

Here, the basis states are (in order, from 1 to 6) $|S_{LL}\rangle$, $|S_{RR}\rangle$, $|S_0\rangle$, $|T_{\uparrow\uparrow}\rangle$, $|T_{\downarrow\downarrow}\rangle$ and $|T_0\rangle$, where $|S_{LL}\rangle$ ($|S_{RR}\rangle$) denotes the state where both electrons are in the left (right) dot with anti-parallel spin (a singlet), $|S_0\rangle$ the singlet state when the two electrons are delocalized one per dot, $|T_{\uparrow\uparrow}\rangle$ and $|T_{\uparrow\uparrow}\rangle$ the spin-polarized triplet states with one electron per dot and, lastly, $|T_0\rangle$ is the triplet state when the two electrons are delocalized one per dot. Please notice that the triplet states

($|T_{LL}\rangle$ and $|T_{RR}\rangle$, both polarized or anti-parallel) are much higher in energy and for this reason are ignored. Back to the Hamiltonian, U is the charging energy (i.e. the coulomb repulsion between two electrons when they share the same dot), ε is the DQD detuning (i.e. the difference between the electro-chemical potential in the two dots), t is the tunneling coupling between the two dots and B_z is an external applied magnetic field.

1. The triplet state $|T_0\rangle$ is an eigenstate of H. The global offset in Eq. (2) was chosen so that the eigenenergy of $|T_0\rangle$ is 0. The exchange splitting J between the energetically lowest singlet state and $|T_0\rangle$ is a very important quantity, because it can be used to implement quantum gates. Assuming that $|\varepsilon| < U$ and $\sqrt{2}t \ll U \pm \varepsilon$, which normally applies to DQDs when detuning is relatively small, show that the formula:

$$J \approx \frac{4t^2 U}{U^2 - \varepsilon^2} \tag{3}$$

   can be derived via Schrieffer-Wolff transformation.

Hint: One block of the Hamiltonian is already diagonal, so diagonalize only the remaining one.
Reminder about Schrieffer-Wolff transformation: Consider a quantum system evolving under the perturbed Hamiltonian $H = H_0 + V$, where H_0 is purely diagonal in some basis and V is purely off-diagonal in the same basis. The Schrieffer-Wolff transformation is a unitary transformation, which puts the Hamiltonian H into the basis where it is diagonal up to the second order of the perturbation parameter. In other words, we transform H into:

$$H' = e^S H e^{-S} = H + [S, H] + \frac{1}{2}[S, [S, H]] + ..., \tag{4}$$

where we chose S to satisfy $V + [S, H_0] = 0$. Hence, we get:

$$H' = H_0 + \frac{1}{2}[S, V] + O(V^3). \tag{5}$$

As was already mentioned, H' computed this way will be diagonal up to the second order in perturbation parameter. Consequently, we get the approximate exchange splitting J from looking at H' diagonal.