Exercise: Exchange Interaction in Two Level System

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The problem:

Two particles are placed in a non symmetric two site system with energy levels $\pm\epsilon$ and a hopping amplitude per unit time, c. The interaction between the two particles is given by the Hubbard model: When both particles occupy the same site, their interaction energy is u, otherwise it is zero. The goal of this problem is to calculate the exchange interaction energy, following two approaches.

(1) Calculate the exchange interaction, $K = \langle 1, 2|U|2, 1\rangle$, where U is a two body operator.
(2) Calculate the exchange interaction using second order perturbation theory.
(3) Compare the results for small u.

The solution:

(1) In the standard basis, the Hamiltonian of a single particle in a two-level system is given by $\mathcal{H}_1 = \begin{pmatrix} 0 & c \\ c & \epsilon \end{pmatrix}$. The eigenfunctions of this system are

$$|+\rangle = \cos\theta|1\rangle + \sin\theta|2\rangle$$

$$|-\rangle = -\sin\theta|1\rangle + \cos\theta|2\rangle$$

The angle θ is obtained from the precession picture:

$$\tan 2\theta = \frac{2c}{\epsilon}$$

For two particles, we may write that

$$\mathcal{H}_0 = \hat{I} \otimes \mathcal{H}_1 + \mathcal{H}_1 \otimes \hat{I} = \begin{pmatrix} 0 & c & c & 0 \\ c & \epsilon & 0 & c \\ c & 0 & \epsilon & c \\ 0 & 0 & c & 2\epsilon \end{pmatrix}$$

Adding the Hubbard interaction

$$\begin{pmatrix} u & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & u \end{pmatrix}$$

we obtain the Hamiltonian:

$$\mathcal{H} = \mathcal{H}_0 + U = \begin{pmatrix} u & c & c & 0 \\ c & \epsilon & 0 & c \\ c & 0 & \epsilon & c \\ 0 & c & c & 2\epsilon + u \end{pmatrix}$$

The unperturbed eigenfunctions are $|++\rangle, |+-\rangle, |-+\rangle, |--\rangle$

$$|++\rangle = \cos^2\theta|1,1\rangle + \sin^2\theta|2,2\rangle + \sin\theta\cos\theta(|1,2\rangle + |2,1\rangle)$$

$$|+-\rangle = \sin\theta\cos\theta(-|1,1\rangle + |2,2\rangle) + \cos^2\theta|1,2\rangle - \sin^2\theta|2,1\rangle$$

$$|-+\rangle = \sin\theta\cos\theta(-|1,1\rangle + |2,2\rangle) - \cos^2\theta|1,2\rangle + \sin^2\theta|2,1\rangle$$
$$|--\rangle = \sin^2\theta|1,1\rangle + \cos^2\theta|2,2\rangle - \sin\theta\cos\theta(|1,2\rangle + |2,1\rangle)$$

The exchange interaction is defined as $K = \langle -+|U|+-\rangle$:

$$K = \frac{u}{2}\sin^2 2\theta$$

After some trigonometric algebra, we arrive at

$$K = u\frac{2c^2}{\epsilon^2 + 4c^2}$$

(2) Consider for a moment the entire system, including the spin of the electrons. In this case there are six possible states:

$$\{|1\uparrow,2\uparrow\rangle, |1\uparrow,1\downarrow\rangle, |1\uparrow,2\downarrow\rangle, |1\downarrow,2\uparrow\rangle, |2\uparrow,2\downarrow\rangle, |1\downarrow,2\downarrow\rangle\}$$

Since the interaction doesn't have any effect on spin, the first and last states are uncoupled. This leaves us with four states and the hamiltonian is the same as in (1). The general Hamiltonian:

$$\mathcal{H}_{6x6} = \begin{pmatrix} \epsilon & 0 & 0 & 0 & 0 & 0 \\ 0 & u & c & c & 0 & 0 \\ 0 & c & \epsilon & 0 & c & 0 \\ 0 & c & 0 & \epsilon & c & 0 \\ 0 & 0 & c & c & 2\epsilon + u & 0 \\ 0 & 0 & 0 & 0 & 0 & \epsilon \end{pmatrix}$$

The reduced 4x4 Hamiltonian

$$\mathcal{H}_{4x4} = \begin{pmatrix} u & c & c & 0 \\ c & \epsilon & 0 & c \\ c & 0 & \epsilon & c \\ 0 & c & c & 2\epsilon + u \end{pmatrix}$$

In order to get rid of the degeneracy, we transform to the following basis

$$|1\uparrow,1\downarrow\rangle, |S\rangle, |A\rangle, |2\uparrow,2\downarrow\rangle$$

in which the Hamiltonian becomes

$$\widetilde{\mathcal{H}} = \begin{pmatrix} u & \sqrt{2}c & 0 & 0 \\ \sqrt{2}c & \epsilon & 0 & \sqrt{2}c \\ 0 & 0 & \epsilon & 0 \\ 0 & \sqrt{2}c & 0 & 2\epsilon + u \end{pmatrix}$$

It is now evident that there is one uncoupled state (the anti-symmetric state), with energy ϵ. The remaining three energies, calculated using second order perturbation theory are

$$E_1 = u - \frac{2c^2}{\epsilon - u} - \frac{2c^2}{2\epsilon}$$

$$E_2 = \epsilon + \frac{2c^2}{\epsilon - u} - \frac{2c^2}{\epsilon + u}$$

$$E_3 = \epsilon$$

$$E_4 = 2\epsilon + u + \frac{2c^2}{\epsilon + u} + \frac{2c^2}{2\epsilon}$$

(3) For small u, the splitting in energy $\Delta E = \frac{E_2 - E_3}{2}$ is

$$\Delta E = u\frac{2c^2}{\epsilon^2}$$

This is in agreement with the result of (1) when the coupling, c, is also weak (this is required, if we want to justify using second order perturbation theory, as in (2)).