Ex1346: A particle in a double well coupeld to a higher level

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The problem:
Assume a particle in a symmetric double well, in which the hopping amplitude from site "1" to site "2" is c_0. In addition, assume a site "0" with the potential energy ϵ_0 which is much greater than c_1 and c_2 the hopping amplitudes from "0" to "1" and "2" respectively. The main goal is to find the effective 2X2 Hamiltonian, that describes the particle in the double well. To achieve the main goal, one must work in a new basis consists of quantum states "C" and "D" which are superpositions of the states "1" and "2". In sections 1-3, assume hopping amplitude between sites $c_0 = 0$.

1. Define a dark state "D", who's coupling to the state "0" is zero.
2. Define a state "C" orthogonal to "D" and find the coupling

   $\langle 0|H|C\rangle$

3. Determine the energies of the states "C" and "D" using perturbation theory.
4. Find the effective 2X2 Hamiltonian that describes the particle in the standard basis.
5. For which value of c0, the particle's eigen state would be located in a single site?

Guidance:

- The answer at section 3 defines an effective Hamiltonian

  $$\hat{\mathcal{H}} = \begin{pmatrix} E_D & 0 \\ 0 & E_C \end{pmatrix}$$

- The answer at section 4 is the same Hamiltonian in the standard basis, represented by a non diagonal matrix.
- At section 4 the coupling c_0 needs to be added to the Hamiltonian.
- the answer at section 5 is derived from observing the Hamiltonian found at section 4.

The solution:

(1) The Hamiltonian is:

$$\hat{\mathcal{H}} = \begin{pmatrix} \epsilon_0 & c_1 & c_2 \\ c_1 & 0 & 0 \\ c_2 & 0 & 0 \end{pmatrix}$$

And "D" is a superposition of "1" and "2":

$$|D\rangle = a|1\rangle + b|2\rangle$$

For no coupling, we demand:

$$0 = \langle 0|H|D\rangle = a\langle 0|H|1\rangle + b\langle 0|H|2\rangle$$

thus

$$(i)\ ac_1 + bc_2 = 0$$

Demanding a normalized vector requires:

$$(ii)\ a^2 + b^2 = 1$$

By solving the two equation system we get

$$|D\rangle = \frac{1}{\sqrt{c_1^2 + c_2^2}}(c_2|1\rangle - c_1|2\rangle) = \frac{1}{\sqrt{c_1^2 + c_2^2}} \begin{pmatrix} c_2 \\ -c_1 \end{pmatrix}$$

(2) For orthogonality:

$$\langle C|D\rangle = 0$$

If we chose

$$|C\rangle = \frac{1}{\sqrt{c_1^2 + c_2^2}}(c_1|1\rangle + c_2|2\rangle) = \frac{1}{\sqrt{c_1^2 + c_2^2}} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

Then

$$\langle C|D\rangle = \frac{1}{c_1^2 + c_2^2}(c_1c_2 - c_1c_2) = 0$$

As required.

To find the coupling of "C" to "0", we calculate:

$$\langle 0|H|C\rangle = \langle 0|H| \left(\frac{1}{\sqrt{c_1^2 + c_2^2}}(c_1|1\rangle + c_2|2\rangle) \right) = \frac{1}{\sqrt{c_1^2 + c_2^2}} \left(c_1\langle 0|H|1\rangle + c_2\langle 0|H|2\rangle\right)$$

And finaly, recalling the known coupling of "0" to "1" and "2":

$$\langle 0|H|C\rangle = \sqrt{c_1^2 + c_2^2}$$

(3) The Hamiltonian in the new basis can be written as a sum of the perturbated and unperturbated parts

$$H_{0,C,D} = \begin{pmatrix} \epsilon_0 & \sqrt{c_1^2 + c_2^2} & 0 \\ \sqrt{c_1^2 + c_2^2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} \epsilon_0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & \sqrt{c_1^2 + c_2^2} & 0 \\ \sqrt{c_1^2 + c_2^2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Since we only have a perturbation for the upper left block of the Hamiltonian, We will use perturbation theory just for this block:

$$H_{0,c} = \begin{pmatrix} \epsilon_0 & 0 \\ 0 & 0 \end{pmatrix} + \sqrt{c_1^2 + c_2^2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Since $c_1, c_2 << \epsilon_0$, perturbation theory method converges
and we get

$$E_d{}^{[0]} = 0$$

$$E_d{}^{[1]} = 0$$
$$E_d{}^{[2]} = 0$$
$$E_d = E_d{}^{[0]} + E_d{}^{[1]} + E_d{}^{[2]} = 0;$$

$$E_c{}^{[0]} = 0$$
$$E_c{}^{[1]} = 0$$
$$E_c{}^{[2]} = c_1^2 + c_2^2$$
$$E_c = E_c{}^{[0]} + E_c{}^{[1]} + E_c{}^{[2]} = -\frac{c_1^2 + c_2^2}{\epsilon_0}$$

$$E_0{}^{[0]} = \epsilon_0$$
$$E_0{}^{[1]} = 0$$
$$E_0{}^{[2]} = \frac{c_1^2 + c_2^2}{\epsilon_0}$$
$$E_0 = E_0{}^{[0]} + E_0{}^{[1]} + E_0{}^{[2]} = \epsilon_0 + \frac{c_1^2 + c_2^2}{\epsilon_0}$$

(4) Let A and B define the standard basis and the new basis respectively.

$$A = \{|0\rangle, |1\rangle, |2\rangle\}$$
$$B = \{|0\rangle, |C\rangle, |D\rangle\}$$

$$\langle A_i|H|A_j\rangle = \langle A_i|B_n\rangle\langle B_i|H|B_j\rangle\langle B_m|A_j\rangle$$

where $\langle B_i|H|B_j\rangle$ is an element in the diagonal Hamiltonian we calculeted for "D","C","0" basis, and $|B_j\rangle\langle B_m|$ is the projection operator to the B basis.
Notice $T = |B_n\rangle\langle B_m|$ is a unitary and Hermitian operator:

$$T = T^\dagger$$
$$TT^\dagger = \mathbf{1}$$

Therefore

$$T = T^{-1}$$

And

$$H = \frac{1}{\sqrt{c_1^2 + c_2^2}} \begin{pmatrix} \sqrt{c_1^2 + c_2^2} & 0 & 0 \\ 0 & c_1 & c_2 \\ 0 & c_2 & -c_1 \end{pmatrix} \frac{c_1^2 + c_2^2}{\epsilon_0} \begin{pmatrix} 1 + \frac{\epsilon_0^2}{c_1^2 + c_2^2} & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \frac{1}{\sqrt{c_1^2 + c_2^2}} \begin{pmatrix} \sqrt{c_1^2 + c_2^2} & 0 & 0 \\ 0 & c_1 & c_2 \\ 0 & c_2 & -c_1 \end{pmatrix}$$

$$H_{1,2} = \frac{1}{\epsilon_0} \begin{pmatrix} -c_1^2 & -c_1 c_2 \\ -c_1 c_2 & -c_2^2 \end{pmatrix} + \begin{pmatrix} 0 & c_0 \\ c_0 & 0 \end{pmatrix}$$

$$H_{1,2} = \frac{1}{\epsilon_0} \begin{pmatrix} -c_1^2 & -c_1 c_2 + \epsilon_0 c_0 \\ -c_1 c_2 + \epsilon_0 c_0 & -c_2^2 \end{pmatrix}$$

(5) To make the eigen states be single sites we demand that the Hamiltonian will be diagonal for the standard basis. (the eigen vectors of the standard basis are single sites).
Thus-

$$c_0 = \frac{c_1 c_2}{\epsilon_0}$$