E1472: Three site system in a row, Dynamics

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The problem:

A particle in a three site system is described using the standard basis: $|1\rangle, |2\rangle, |3\rangle$, with the Hamiltonian

$$\mathcal{H} = \begin{pmatrix} 0 & c_a & 0 \\ c_a & 0 & c_b \\ 0 & c_b & 0 \end{pmatrix}, \qquad c_a = c\cos(\theta),\ c_b = c\sin(\theta)$$

The particle is prepared in the first site at t=0.
Express your answer with θ, c.
To solve clause (1) find the roots of the polynomial equation (very simple formula).

(1) Find the eigenvalues of the Hamiltonian: E_0, E_+, E_-.

(2) Using the standad basis write the eigenstates $|0\rangle, |+\rangle, |-\rangle$.

(3) Write the intial state in the energy basis.

(4) Write an expression for $P(t)$, the probability of finding the particle in the first site after a time period of t.

(5) Write and expression for $I(t)$, the expectation vaule of the current which is measured between sites $|2\rangle$ and $|3\rangle$ at time t.

The solution:

(1) Using diagonalization, we solve the equation,

$$det(\mathcal{H} - \lambda\mathbb{I}) = 0$$

thus finding the eigenvalues:

$$E_0 = 0 \qquad E_\pm = \pm c$$

(2) Solving $(\mathcal{H} - \lambda_i\mathbb{I})$ we find that the eigenstates of the Hamiltonian are:

$$|0\rangle = \begin{pmatrix} \sin\theta \\ 0 \\ -\cos\theta \end{pmatrix}, \qquad |+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} \cos\theta \\ 1 \\ \sin\theta \end{pmatrix}, \qquad |+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} \cos\theta \\ -1 \\ \sin\theta \end{pmatrix}$$

and written in the dirac notation:

$$|0\rangle = (\sin\theta|1\rangle - \cos\theta|3\rangle)$$

$$|+\rangle = \frac{1}{\sqrt{2}}(\cos\theta|1\rangle + |2\rangle + \sin\theta|3\rangle)$$

$$|-\rangle = \frac{1}{2}(\cos\theta|1\rangle - |2\rangle + \sin\theta|3\rangle)$$

(3) Expressing the initial state in the energy basis we get:

$$|1\rangle = \sin\theta|0\rangle + \frac{1}{\sqrt{2}}\cos\theta(|+\rangle + |-\rangle)$$

(4) To find P(t) we use the formula : $P(t) = |\langle 1|\psi(t)\rangle|^2$

First we need to define $\psi(t)$

$$\Phi_t = |1\rangle \mathrm{e}^{-iE_1 t} = \sin\theta|0\rangle + \frac{1}{\sqrt{2}}\cos\theta(|+\rangle\mathrm{e}^{-ict} + |-\rangle\mathrm{e}^{ict})$$

then $\psi(t) = \begin{pmatrix} \langle 1|\Phi_t\rangle \\ \langle 2|\Phi_t\rangle \\ \langle 3|\Phi_t\rangle \end{pmatrix}$ giving us:

$$\psi(t) = \begin{pmatrix} \sin^2\theta + \cos^2\theta\cos(ct) \\ \cos\theta(-i\sin(ct)) \\ -\sin\theta\cos\theta(1-\cos(ct)) \end{pmatrix}$$

$$P(t) = |\sin^2\theta + \frac{1}{2}\cos^2\theta\mathrm{e}^{-ict} + \frac{1}{2}\cos^2\theta\mathrm{e}^{ict}|^2 = |\sin^2\theta + \cos^2\theta\cos(ct)|^2$$

(5) In order to find I(t) we first must find the operator $\hat{I}$ we can do that in two ways :

1. The current operator is defined as $\hat{I} = \frac{\partial\hat{\mathcal{H}}}{\partial\phi}|_{\phi=0}$, in order to do that we must place a test flux between sites $|2\rangle\, and\, |3\rangle$ giving us

$$\hat{\mathcal{H}} = \begin{pmatrix} 0 & c_a & 0 \\ c_a & 0 & c_b\mathrm{e}^{i\phi} \\ 0 & c_b\mathrm{e}^{-i\phi} & 0 \end{pmatrix}$$

   Using this $\mathcal{H}\, we\, can\, find\, \hat{I}$:

$$\hat{I} = \frac{\partial\hat{\mathcal{H}}}{\partial\phi}|_{\phi=0} = i\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & c_b \\ 0 & -c_b & 0 \end{pmatrix}$$

2. Using the general site model:

$$\hat{I}_{i\to j} = -i\left[\hat{\mathcal{H}}, \hat{P}^i\right] = -i[|j\rangle\mathcal{H}_{ji}\langle i| - |i\rangle\mathcal{H}_{ij}\langle j|]$$

$$\hat{I}_{2\to 3} = i\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & c_b \\ 0 & -c_b & 0 \end{pmatrix}$$

To find the expectation value of $\hat{I}_{2\to3}(t)$:

$$\langle\psi(t)|\hat{I}|\psi(t)\rangle = \begin{pmatrix}\psi_1, & \psi_2, & \psi_3\end{pmatrix} \cdot \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & ic_b \\ 0 & -ic_b & 0 \end{pmatrix} \cdot \begin{pmatrix}\psi_1 \\ \psi_2 \\ \psi_3\end{pmatrix} = 2C_b \cos^2\theta \sin\theta \sin(ct)(1-\cos(ct))$$

With the use of a simple trigonometric identity we finally get:

$$\langle I(t)\rangle = \frac{1}{2}c|\sin\theta|^2 \sin(ct)(1-\cos(ct))$$