E1380: system with three sites

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The problem:

A system with three sites described by the hamiltonian

$$\hat{\mathcal{H}} = \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}$$

and the position matrix:

$$\hat{\mathcal{X}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

The particle's charge is e.

(1) Write the Hamiltonian if we add a magnetic flux Φ, through the ring which connects the sites.
(2) Define the current operator using the formula $I = -\frac{dH}{d\Phi}$. Assume from now on the flux is zero.
(3) Write in the standard basis the eigenstates and the energies eigenvalues. Note that the hamiltonian is symmetrical.

The particle is prepared in the "first" site.
(4) Calculate the probability $P(t)$ to find the particle in the first site after time t.
(5) Calculate the current $\langle I \rangle_t$ which flows through the ring.

The solution:

(1) The Hamiltonian is

$$\hat{\mathcal{H}} = \begin{pmatrix} 2 & -1 & -e^{-i\phi} \\ -1 & 2 & -1 \\ -e^{i\phi} & -1 & 2 \end{pmatrix}$$

and the phase is $\phi = e\Phi$

(2) The current when $\Phi = 0$ is:

$$I = -\frac{dH}{d\Phi} = e \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}$$

(3) The momentum eigenvalues are: $k_0 = 0$, $k_+ = \frac{2\pi}{3}$, $k_- = -\frac{2\pi}{3}$ and the eigenstates are (because the hamiltonian is symmetrical to translations its eigenstates are the momentum states):

$$|k_0\rangle = \frac{1}{\sqrt{3}}(|0\rangle + |1\rangle + |2\rangle)$$

$$|k_+\rangle = \frac{1}{\sqrt{3}}(|0\rangle + \mathrm{e}^{i\frac{2\pi}{3}}|1\rangle + \mathrm{e}^{-i\frac{2\pi}{3}}|2\rangle)$$

$$|k_-\rangle = \frac{1}{\sqrt{3}}(|0\rangle + \mathrm{e}^{-i\frac{2\pi}{3}}|1\rangle + \mathrm{e}^{i\frac{2\pi}{3}}|2\rangle)$$

We can write the hemiltonian as:

$$\hat{H} = 2\hat{I} - (\hat{D} + \hat{D}^\dagger) = 2\hat{I} - (\mathrm{e}^{-i\hat{p}} + \mathrm{e}^{i\hat{p}}) = 2\hat{I} - 2cos(\hat{p})$$

So the energies are:

$$E_0 = 0$$

$$E_+ = 3$$

$$E_- = 3$$

(4) The state of a particle in the "first" site written in the momentum basis is:

$$|0\rangle = \frac{1}{\sqrt{3}}(|k_0\rangle + |k_+\rangle + |k_-\rangle)$$

The particle was prepared in such state, so it's wave function at time t would be:

$$|\psi(t)\rangle = \frac{1}{\sqrt{3}}(|k_0\rangle + \mathrm{e}^{-i\omega t}(|k_+\rangle + |k_-\rangle))$$

where $\omega = E_+ = E_- = 3$.
The probability to find the particle at the "first" site after time t is:

$$P(t) = |\langle 0|\psi(t)\rangle|^2 = |\frac{1}{3}(1 + \mathrm{e}^{-i\omega t} + \mathrm{e}^{-i\omega t})|^2 = \frac{1}{9}(5 + 4\cos(\omega t))$$

(5) Lets write the wave function in the position basis:

$$|\psi(t)\rangle = \frac{1}{3}((1 + 2\mathrm{e}^{-i\omega t})|0\rangle + (1 - \mathrm{e}^{-i\omega t})|1\rangle - \mathrm{e}^{-i\omega t})|2\rangle)$$

The current operator is already written in position basis, so by simple multiplication we get:

$$\langle I\rangle_t = \langle\psi(t)|I|\psi(t)\rangle = \frac{2}{9}e\sin\omega t$$