# 1450: Current in a two site system

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**The problem:**

A particle is placed in a site 1 of a symmetric two sites system and oscillates coherently between the two sites. The hopping amplitude per unit time is $c$. The operator $\hat{N} = |1\rangle\langle 1|$ is defied such that its expected value is the probability to find the particle in the first site. The operator $\hat{I}$ is defined from the Operator's Rate of Change formula (see Sec. [8.4] in the lecturer's Lecture Notes) for the operator $\hat{N}$.

(1) Write the matrix form of the Hamiltonian $\hat{\mathcal{H}}$ and the operator $\hat{N}$.
(2) Write the definition of the operator $\hat{I}$ using the operators $\hat{\mathcal{H}}$ and $\hat{N}$.
(3) Write the matrix form of the operator $\hat{I}$.
(4) Find the expectation value of the operator $\hat{I}$ after time $t$.
(5) Find the variance of the operator $\hat{I}$ after time $t$. Reminder: $\mathrm{Var}(x) = \left\langle \hat{I}^2 \right\rangle - \left\langle \hat{I} \right\rangle^2$.

In the Heisenberg picture, the operator $\hat{I}(t)$ is defined as $\hat{I}(t) = U^{-1}(t)\hat{I}_s U(t)$, such that $\hat{I}_s$ is the current operator in the Schrödinger picture.

(6) Write the matrix form of the operator $\hat{I}(t)$ and represent it as a sum of Pauli Matrices.

$\hat{Q}(t)$ is a counting operator. It is defined as $\hat{Q}(t) = \int_0^t \hat{I}(t')\mathrm{d}t$.

(7) What is the expectation value of $\hat{Q}(t)$ after a period?
(8) What is the expectation value of $\hat{Q}(t)$ after a half of a period?

**The solution:**

(1) The Hamiltonian in the position basis is

$$\mathcal{H} = \begin{pmatrix} \epsilon & c \\ c^* & \epsilon \end{pmatrix}$$

We can now shift the energy by a constant such that $\epsilon = 0$ which gives us:

$$\mathcal{H} = \begin{pmatrix} 0 & c \\ c^* & 0 \end{pmatrix}$$

As the system is symmetric $c = c^* = \mathrm{Re}\,(c)$, one gets a real Hamiltonian.

$$\mathcal{H} = \begin{pmatrix} 0 & c \\ c & 0 \end{pmatrix} = c\sigma_x$$

The eigenstates of the Hamiltonian are the states which are even or odd with respect to reflection, so we define:

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

Which has an eigenvalue of $\mathcal{H}|+\rangle = E|+\rangle = c|+\rangle$, and

$$|-\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)$$

Which has an eigenvalue of $\mathcal{H}|-\rangle = E|-\rangle = -c|-\rangle$.

(2) From the definition of $\hat{I}$: $\hat{I} \equiv \frac{d}{dt}\left\langle \hat{N} \right\rangle$. According to the Operator's Rate of Change formula:

$$\hat{I} = i\left[\hat{\mathcal{H}}, \hat{N}\right] + \frac{\partial \hat{N}}{\partial t}$$

Since $\hat{N}$ is not a function of $t$: $\frac{\partial \hat{N}}{\partial t} = 0$.

(3) In order to find the matrix form of $\hat{I}$ one must calculate the commutation relation

$$\left[\hat{\mathcal{H}}, \hat{N}\right] = \begin{pmatrix} 0 & -c \\ c & 0 \end{pmatrix}$$

so

$$\hat{I} = \begin{pmatrix} 0 & -ic \\ ic & 0 \end{pmatrix} = c\sigma_y$$

(4)
The initial state in the new basis is:

$$|\psi(t=0)\rangle = |1\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$$

The time dependant wave function can be written as:

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left(\mathrm{e}^{-ict}|+\rangle + \mathrm{e}^{-i(-c)t}|-\rangle\right) = (\cos(ct)|1\rangle - i\sin(ct)|2\rangle)$$

and so the expectation value of $\hat{I}$ is:

$$\left\langle \hat{I} \right\rangle = \left\langle \psi_{(t)} \middle| \hat{I} \middle| \psi_{(t)} \right\rangle = -\left(\cos(ct), i\sin(ct)\right)\begin{pmatrix} 0 & -ic \\ ic & 0 \end{pmatrix}\begin{pmatrix} \cos(ct) \\ -i\sin(ct) \end{pmatrix} = -c\sin(2ct)$$

(5) The variance of $\hat{I}$ after time $t$ is $\mathrm{Var}(x) = \left\langle \hat{I}^2 \right\rangle - \left\langle \hat{I} \right\rangle^2$.
It is easy to find $\left\langle \hat{I} \right\rangle^2$ from (4):

$$\left\langle \hat{I} \right\rangle^2 = c^2\sin^2(2ct)$$

We compute $\left\langle \hat{I}^2 \right\rangle$ by definition. Simple matrix multiplication gives $\hat{I}^2 = \begin{pmatrix} c^2 & 0 \\ 0 & c^2 \end{pmatrix}$ and so

$$\left\langle \hat{I}^2 \right\rangle = \left\langle \psi_{(t)} \middle| \hat{I}^2 \middle| \psi_{(t)} \right\rangle = \left(\cos(ct), i\sin(ct)\right)\begin{pmatrix} c^2 & 0 \\ 0 & c^2 \end{pmatrix}\begin{pmatrix} \cos(ct) \\ -i\sin(ct) \end{pmatrix} = c^2$$

By definition

$$\mathrm{Var}(x) = \left\langle \hat{I}^2 \right\rangle - \left\langle \hat{I} \right\rangle^2 = c^2 - c^2 \sin^2(2ct) = c^2 \cos^2(ct)$$

(6) From the definition of the Hamiltonian as the generator of the movement in time $\hat{U}(t) = \mathrm{e}^{-i\hat{\mathcal{H}}t}$. $\hat{\mathcal{H}}t = \begin{pmatrix} 0 & ct \\ ct & 0 \end{pmatrix} = ct\sigma_x;\sigma_x = \frac{1}{2}S_x$, where $\sigma_x$ is a Pauli matrix.

Using the formula, $\mathrm{e}^{-i\Phi S_n} = \cos(\frac{\Phi}{2})\hat{1} - i\sin(\frac{\Phi}{2})\sigma_n$ one gets $\hat{U}(t) = \begin{pmatrix} \cos(ct) & -i\sin(ct) \\ -i\sin(ct) & \cos(ct) \end{pmatrix}$.

$\hat{U}(t)$ is a unitary operator, so $\hat{U}^{-1}(t) = \hat{U}(t)$. Therefore,

$$\hat{I}(t) = \hat{U}^{-1}(t)\hat{I}_s(t)\hat{U}(t) = \begin{pmatrix} \cos(ct) & i\sin(ct) \\ i\sin(ct) & \cos(ct) \end{pmatrix} \begin{pmatrix} 0 & -ic \\ ic & 0 \end{pmatrix} \begin{pmatrix} \cos(ct) & -i\sin(ct) \\ -i\sin(ct) & \cos(ct) \end{pmatrix} =$$

$$\begin{pmatrix} -c\sin(2ct) & -ic\cos(2ct) \\ i\cos(2ct) & c\sin(2ct) \end{pmatrix} = \sigma_y(c\cos(2ct)) - \sigma_z(c\sin(2ct))$$

(7) Before any computation which includes the integral of an operator, one has to understand what it is. The integral of the linear operator $\hat{A}$ in the interval $[t_1, t_2]$ is defined as the limit of the Riemann sum $\sum_{i=0}^{n-1} \hat{A}(\xi_i)(x_{i+1} - x_i)$ such that $\xi_i \in (x_{i+1} - x_i)$, as the partitions of the interval get finer. Note that for every two linear operators represented as matrices $\hat{B}$ and $\hat{C}$, $\left[\hat{B} + \hat{C}\right]_{mn} = \left[\hat{B}_{mn} + \hat{C}_{mn}\right]$. Therefore, $\left[\sum_{i=0}^{n-1} \hat{A}(\xi_i)(x_{i+1} - x_i)\right]_{mn} = \left[\sum_{i=0}^{n-1} \hat{A}(\xi_i)_{mn}(x_{i+1} - x_i)\right]$. As a result the integral of the linear operator $\hat{A}$ is a new operator that each of its matrix elements is an integral of the elements in the same place at $\hat{A}$.
Therefore,

$$\int \hat{I}(t')\,\mathrm{d}\,t' = \frac{1}{2}\begin{pmatrix} \cos(2ct) & -i\sin(2ct) \\ i\sin(2ct) & \cos(2ct) \end{pmatrix}$$

One can easily see that $T = \frac{\pi}{c}$. in order to calculate the integral $\int_0^T \hat{I}(t')\,\mathrm{d}\,t'$ one needs to substitute the lower and upper limit of this integral in the formula for $\int \hat{I}(t')\,\mathrm{d}\,t'$. After the substitution one gets

$$\hat{Q}(t = T) = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Therefore, without any further calculation, $\left\langle \hat{Q}(t = T) \right\rangle = 0$.

(8) The calculation of $\int_0^{\frac{T}{2}} \hat{I}(t')\,\mathrm{d}\,t'$ is done in the same way as in the previous part, just with the upper limit $t = \frac{T}{2}$.

$$\hat{Q}(t = \frac{T}{2}) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

Therefore,

$$\left\langle \hat{Q}(t = \frac{T}{2}) \right\rangle = \left[(\cos(ct), i\sin(ct)) \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \cos(ct) \\ -i\sin(ct) \end{pmatrix}\right] \Big|_{t=\frac{T}{2}} = 1$$