

## EXERCISE 16

### Two alternative expressions for $\langle H \rangle$

A quantum system with the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

is described by the wave function

$$\Psi(x, t) = c_1 \psi_1(x) e^{-iE_1 t/\hbar} + c_2 \psi_2(x) e^{-iE_2 t/\hbar} + c_3 \psi_3(x) e^{-iE_3 t/\hbar} + \dots$$

The stationary state energies,  $E_n$ , are all distinct and arranged in ascending order

$$E_1 < E_2 < E_3 < \dots$$

The stationary state functions, satisfying  $\hat{H}\psi_n = E_n\psi_n$ , are normalized to unity.

On the one hand, an energy measurement on the system returns the value  $E_1$  with probability  $|c_1|^2$ , the value  $E_2$  with probability  $|c_2|^2$ , the value  $E_3$  with probability  $|c_3|^2$ , and so on. Consequently, the energy expectation value can be expressed as

$$\langle H \rangle = E_1 |c_1|^2 + E_2 |c_2|^2 + E_3 |c_3|^2 + \dots$$

On the other hand, according to the general rule for expectation values, we have

$$\langle H \rangle = \int_{-\infty}^{+\infty} \Psi^*(x, t) \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \Psi(x, t) dx.$$

Demonstrate that these two expressions for the expectation value of the system's energy are equivalent.

## Solution

Let us start from the second expression for the energy expectation value,

$$\langle H \rangle = \int_{-\infty}^{+\infty} \Psi^*(x, t) \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \Psi(x, t) dx,$$

and transform it into the first expression,

$$\langle H \rangle = \sum_n E_n |c_n|^2.$$

Here, the  $n$ -sum is assumed to run over all stationary states of the system.

Using the stationary state expansion

$$\Psi(x, t) = \sum_n c_n \psi_n(x) e^{-iE_n t/\hbar},$$

we write

$$\begin{aligned} \langle H \rangle &= \int_{-\infty}^{+\infty} \Psi^*(x, t) \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \Psi(x, t) dx \\ &= \int_{-\infty}^{+\infty} \left( \sum_k c_k^* \psi_k^*(x) e^{iE_k t/\hbar} \right) \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \left( \sum_n c_n \psi_n(x) e^{-iE_n t/\hbar} \right) dx \\ &= \sum_k \sum_n c_k^* c_n e^{i(E_k - E_n)t/\hbar} \int_{-\infty}^{+\infty} \psi_k^*(x) \left( -\frac{\hbar^2}{2m} \frac{\partial^2 \psi_n(x)}{\partial x^2} + V(x) \psi_n(x) \right) dx. \end{aligned}$$

Taking into account the time-independent Schrödinger equation satisfied by  $\psi_n(x)$ ,

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_n(x)}{\partial x^2} + V(x) \psi_n(x) = E_n \psi_n(x),$$

we obtain

$$\langle H \rangle = \sum_k \sum_n c_k^* c_n e^{i(E_k - E_n)t/\hbar} E_n \int_{-\infty}^{+\infty} \psi_k^*(x) \psi_n(x) dx.$$

Following the strategy used in EXERCISE 15, we split the double sum into diagonal ( $k = n$ ) and off-diagonal ( $k \neq n$ ) parts:

$$\begin{aligned} \langle H \rangle &= \sum_n E_n |c_n|^2 \int_{-\infty}^{+\infty} |\psi_n(x)|^2 dx \\ &\quad + \sum_k \sum_{n \neq k} E_n c_k^* c_n e^{i(E_k - E_n)t/\hbar} \int_{-\infty}^{+\infty} \psi_k^*(x) \psi_n(x) dx. \end{aligned}$$

Then, using the normalization condition,

$$\int_{-\infty}^{+\infty} |\psi_n(x)|^2 dx = 1 \quad (\text{for all } n),$$

and the orthogonality condition (see EXERCISE 14),

$$\int_{-\infty}^{+\infty} \psi_k^*(x)\psi_n(x) dx = 0 \quad (\text{if } k \neq n),$$

we arrive at the sought expression for the energy expectation value:

$$\langle H \rangle = \sum_n E_n |c_n|^2$$