Exercise 14
Determining expansion coefficients from the initial wave function

Consider a one-dimensional quantum system with stationary states

$$\psi_1(x)\,,\ \psi_2(x)\,,\ \psi_3(x)\,,\ \ldots$$

All stationary states are properly normalized:

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

Suppose that the energies of these stationary states are all different and, for concreteness, are arranged in the ascending order:

$$E_1 < E_2 < E_3 < \ldots$$

1. Demonstrate that all stationary states are mutually orthogonal, i.e.

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

2. The completeness property of the stationary states, combined with the linearity of the Schrödinger equation, guarantees that any time-dependent state of the system, $\Psi(x,t)$, can be represented as a superposition of the stationary states:

$$\Psi(x,t) = c_1\psi_1(x)e^{-iE_1t/\hbar} + c_2\psi_2(x)e^{-iE_2t/\hbar} + c_3\psi_3(x)e^{-iE_3t/\hbar} + \ldots$$

   Show that the expansion coefficients c_1, c_2, c_3, ... can be determined from the initial wave function $\Psi(x,0)$ as follows:

$$c_n = \int_{-\infty}^{+\infty} \psi_n^*(x)\Psi(x,0)\, dx\,.$$

Solution

1. Consider an arbitrary pair of stationary state wave functions, $\psi_k(x)$ and $\psi_n(x)$, with $k \neq n$. The wave functions are solutions to the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_k(x)}{dx^2} + V(x)\psi_k(x) = E_k\psi_k(x)\,, \tag{1}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} + V(x)\psi_n(x) = E_n\psi_n(x)\,. \tag{2}$$

Complex conjugating Eq. (1) and then multiplying both sides by $\psi_n(x)$, we get

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_k^*(x)}{dx^2}\psi_n(x) + V(x)\psi_k^*(x)\psi_n(x) = E_k\psi_k^*(x)\psi_n(x)\,.$$

Integrating both sides over x, we obtain

$$-\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\frac{d^2\psi_k^*(x)}{dx^2}\psi_n(x)\,dx + \int_{-\infty}^{+\infty}V(x)\psi_k^*(x)\psi_n(x)\,dx = E_k\int_{-\infty}^{+\infty}\psi_k^*(x)\psi_n(x)\,dx\,. \tag{3}$$

Then, multiplying Eq. (2) by $\psi_k^*(x)$,

$$-\frac{\hbar^2}{2m}\psi_k^*(x)\frac{d^2\psi_n(x)}{dx^2} + V(x)\psi_k^*(x)\psi_n(x) = E_n\psi_k^*(x)\psi_n(x)\,,$$

and integrating both sides over x, we get

$$-\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\psi_k^*(x)\frac{d^2\psi_n(x)}{dx^2}\,dx + \int_{-\infty}^{+\infty}V(x)\psi_k^*(x)\psi_n(x)\,dx = E_n\int_{-\infty}^{+\infty}\psi_k^*(x)\psi_n(x)\,dx\,. \tag{4}$$

Using integration by parts (twice!), we show that the first integral in Eq. (4) is the same as the first integral in Eq. (3):

$$\begin{aligned}\int_{-\infty}^{+\infty}\psi_k^*(x)\frac{d^2\psi_n(x)}{dx^2}\,dx &= -\int_{-\infty}^{+\infty}\frac{d\psi_k^*(x)}{dx}\frac{d\psi_n(x)}{dx}\,dx\\ &= \int_{-\infty}^{+\infty}\frac{d^2\psi_k^*(x)}{dx^2}\psi_n(x)\,dx\,.\end{aligned}$$

In view of this, Eq. (4) can be rewritten as

$$-\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\frac{d^2\psi_k^*(x)}{dx^2}\psi_n(x)\,dx + \int_{-\infty}^{+\infty}V(x)\psi_k^*(x)\psi_n(x)\,dx = E_n\int_{-\infty}^{+\infty}\psi_k^*(x)\psi_n(x)\,dx\,. \tag{5}$$

Now, subtracting Eq. (5) from Eq. (3), we obtain

$$(E_k - E_n) \int_{-\infty}^{+\infty} \psi_k^*(x)\psi_n(x)\,dx = 0\,.$$

Since, as stated in the question, $E_k \neq E_n$ for $k \neq n$, the last equality reduces to the sought orthogonality condition:

$$\boxed{\int_{-\infty}^{+\infty} \psi_k^*(x)\psi_n(x)\,dx = 0}$$

2. Multiplying both sides of the expansion

$$\Psi(x,t) = c_1\psi_1(x)e^{-iE_1t/\hbar} + c_2\psi_2(x)e^{-iE_2t/\hbar} + c_3\psi_3(x)e^{-iE_3t/\hbar} + \ldots$$

by $\psi_n^*(x)$ and integrating them over x, we find

$$\begin{aligned}\int_{-\infty}^{+\infty} \psi_n^*(x)\Psi(x,t)\,dx = c_1e^{-iE_1t/\hbar} &\int_{-\infty}^{+\infty} \psi_n^*(x)\psi_1(x)\,dx \\ &+ c_2e^{-iE_2t/\hbar} \int_{-\infty}^{+\infty} \psi_n^*(x)\psi_2(x)\,dx \\ &+ c_3e^{-iE_3t/\hbar} \int_{-\infty}^{+\infty} \psi_n^*(x)\psi_3(x)\,dx \\ &+ \ldots \end{aligned} \tag{6}$$

In view of the orthogonality condition,

$$\begin{aligned}\int_{-\infty}^{+\infty} \psi_n^*(x)\psi_1(x)\,dx = 0 \quad \text{unless } n = 1\,,\\ \int_{-\infty}^{+\infty} \psi_n^*(x)\psi_2(x)\,dx = 0 \quad \text{unless } n = 2\,,\\ \int_{-\infty}^{+\infty} \psi_n^*(x)\psi_3(x)\,dx = 0 \quad \text{unless } n = 3\,,\\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\end{aligned}$$

Therefore, only a single integral survives in the right-hand side of Eq. (6), which leads to

$$\int_{-\infty}^{+\infty} \psi_n^*(x)\Psi(x,t)\,dx = c_ne^{-iE_nt/\hbar} \int_{-\infty}^{+\infty} \psi_n^*(x)\psi_n(x)\,dx\,.$$

Subsequently, the integral in the right-hand side of the last equation equals one due to the normalization condition:

$$\int_{-\infty}^{+\infty} \psi_n^*(x)\psi_n(x)\,dx = \int_{-\infty}^{+\infty} |\psi_n(x)|^2\,dx = 1\,.$$

This leaves us with

$$\int_{-\infty}^{+\infty} \psi_n^*(x)\Psi(x,t)\,dx = c_n e^{-iE_n t/\hbar}\,.$$

Finally, setting t to zero, we obtain the desired formula for the n^{th} expansion coefficient:

$$\boxed{c_n = \int_{-\infty}^{+\infty} \psi_n^*(x)\Psi(x,0)\,dx}$$