Solution 9

1. Particle in a box

The wave function $\psi(x)$ of an eigenstate in the infinite potential well of width a satisfies the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi\,, \qquad (\psi(0) = \psi(a) = 0)\,.$$

In order for the solutions

$$\psi(x) = A\cos kx + B\sin kx\,, \qquad (k^2 = \frac{2mE}{\hbar^2})$$

to satisfy the boundary conditions, we must have

$$A = 0\,, \qquad ka = n\pi\,, \qquad (n = 1, 2, \dots)\,.$$

Moreover, since states are normalized we have

$$1 = \langle\psi,\psi\rangle = |B|^2\int_0^a \sin^2\frac{n\pi}{a}x dx = |B|^2\frac{a}{2}\,,$$

i.e. $B = \sqrt{2/a}$ (up to a phase). The energy is $E = (\hbar k)^2/2m = (\hbar\pi n)^2/2ma^2$; the ground state thus corresponds to $n = 1$.

(i) Denote the wave function of the ground state in the well of width $a/2$ by $\psi_1^{\frac{a}{2}}(x)$, and the ground and first excited state in the well of width a by $\psi_1^a(x)$ and $\psi_2^a(x)$ respectively. We have

$$\langle\psi_2^a,\psi_1^{\frac{a}{2}}\rangle = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a/2}}\int_0^{a/2}\sin\frac{2\pi}{a}x\cdot\sin\frac{\pi x}{a/2}dx = \frac{2\sqrt{2}}{a}\cdot\frac{a}{2}\cdot\frac{1}{2} = \frac{\sqrt{2}}{2}\,.$$

The corresponding probability is

$$\left|\langle\psi_2^a,\psi_1^{\frac{a}{2}}\rangle\right|^2 = \frac{1}{2}\,. \tag{9}$$

On the other hand,

$$\begin{aligned}\langle\psi_1^a,\psi_1^{\frac{a}{2}}\rangle &= \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a/2}}\int_0^{a/2}\sin\frac{\pi x}{a}\sin\frac{\pi x}{a/2}dx\\ &= \frac{2\sqrt{2}}{a}\frac{a}{\pi}\int_0^{\pi}2\sin^2 y\cos y\,dy = \frac{4\sqrt{2}}{3\pi}\sin^3 y\Big|_0^{\pi} = \frac{4\sqrt{2}}{3\pi}\,.\end{aligned}$$

The corresponding probability is thus

$$\left|\langle\psi_1^a,\psi_1^{\frac{a}{2}}\rangle\right|^2 = \frac{32}{9\pi^2}\,.$$

(ii) The Hamiltonians (energy operators) before and after the shift are

$$H_{a/2} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \qquad \text{on} \quad [0, a/2]\,,$$
$$H_a = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \qquad \text{on} \quad [0, a]\,.$$

Let now $x \in [0, a]$ and denote by $\Theta(x)$ the Heaviside step function. For the wave function

$$\psi(x) = \frac{2}{\sqrt{a}}\sin\frac{2\pi}{a}x\;\Theta(-x+\frac{a}{2}) = \begin{cases} \psi_1^{\frac{a}{2}}(x) = \frac{2}{\sqrt{a}}\sin\frac{2\pi}{a}x\,, & (0 < x < \frac{a}{2}) \\ 0\,, & (\frac{a}{2} < x < a) \end{cases}$$

we have

$$\frac{d\psi}{dx} = \begin{cases} \frac{4\pi}{a\sqrt{a}}\cos\frac{2\pi x}{a}\,, & (0 < x < \frac{a}{2}) \\ 0\,, & (\frac{a}{2} < x < a)\,. \end{cases}$$

This follows from

$$\frac{d}{dx}\Theta(-x+\frac{a}{2}) = -\delta(-x+\frac{a}{2}) = -\delta(x-\frac{a}{2})\,,$$

and $\sin\frac{2\pi}{a}x$ vanishing at $x = a/2$. Similarly, we get

$$\frac{d^2\psi}{dx^2} = \left.\begin{cases} -\frac{8\pi}{a^2\sqrt{a}}\sin\frac{2\pi}{a}x\,, & (0 < x < \frac{a}{2}) \\ 0\,, & (\frac{a}{2} < x < a) \end{cases}\right\} + \frac{4\pi}{a\sqrt{a}}\,\delta\big(x-\frac{a}{2}\big)\,.$$

Hence

$$H_a\psi = H_{a/2}\psi - \frac{\hbar^2}{2m}\frac{4\pi}{a\sqrt{a}}\delta\big(x-\frac{a}{2}\big)$$

and

$$\langle\psi, H_a\psi\rangle = \langle\psi, H_{a/2}\psi\rangle - \frac{\hbar^2}{2m}\frac{4\pi}{a\sqrt{a}}\,\bar{\psi}\big(\frac{a}{2}\big) = \langle\psi, H_{a/2}\psi\rangle\,.$$

The expectation value of the energy is conserved in the present case. The variance is $\langle\psi, (H_a - \langle\psi, H_a\psi\rangle)^2\psi\rangle = \langle\psi, H_a^2\psi\rangle - \langle\psi, H_a\psi\rangle^2$; and we have

$$\langle\psi, H_a^2\psi\rangle = \langle(H_a\psi), (H_a\psi)\rangle = \infty\,;$$

i.e. the variance is divergent. This follows from the δ-function not being square-integrable:

$$\int_0^a \delta(x-\frac{a}{2})\delta(x-\frac{a}{2})\,\mathrm{d}x = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_0^a \mathrm{e}^{\mathrm{i}p(x-\frac{a}{2})}\delta(x-\frac{a}{2})\,\mathrm{d}x\,\mathrm{d}p = \frac{1}{2\pi}\int_{-\infty}^{\infty} 1\,\mathrm{d}p = \infty\,.$$

2. Transfer matrix and scattering matrix

(i) We can write equation (2) as

$$(\psi' - \mathrm{i}A(x)\psi)' = \mathrm{i}A\psi' + A^2\psi + (V-E)\psi\,.$$

Hence

$$\begin{aligned} j' &= 2\mathrm{Im}\big(\bar{\psi}'(\psi' - \mathrm{i}A\psi) + \bar{\psi}(\psi' - \mathrm{i}A\psi)'\big) \\ &= 2\mathrm{Im}(\bar{\psi}'\psi' - \mathrm{i}\bar{\psi}'A\psi + \mathrm{i}\bar{\psi}A\psi' + \bar{\psi}A^2\psi + \bar{\psi}(V-E)\psi) = 0\,, \end{aligned}$$

since the second and third term are complex conjugated w.r.t. each other, and the rest is real.

(ii) There are two linearly independent solutions of the second order differential equation (2) on $\mathbb{R}$ since for each x_0, the values $\psi(x_0)$, $\psi'(x_0)$ determine the solution. The set of solutions is thus two-dimensional, and on the considered domains, the functions $\{e^{\pm ikx}\}_{x\le a}$ and $\{e^{\pm ikx}\}_{x\ge b}$ constitute bases respectively. By (i), we have $j(a) = j(b)$. Using $\psi' = ik(a_+e^{ikx} - a_-e^{-ikx})$, we get $j(x) = 2k(|a_+|^2 - |a_-|^2)$, $(x \le a)$ and similarly for $x \ge b$, thus

$$|a_+|^2 - |a_-|^2 = |a'_+|^2 - |a'_-|^2 \,. \tag{10}$$

This equality of quadratic forms in (a'_+, a'_-) corresponds to the equality of the associated hermitian matrices (4).

(iii) By (5, 6),

$$T\begin{pmatrix} t \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ r \end{pmatrix}, \qquad T\begin{pmatrix} r' \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ t' \end{pmatrix}.$$

With this, one can form the $2 \times 2 = 4$ matrix elements of equation (4):

$$\begin{aligned} 1 - |r|^2 &= |t|^2 \,, & -\bar{r}t' &= \bar{t}r' \,, \\ -\bar{t}'r &= \bar{r}'t \,, & -|t'|^2 &= |r'|^2 - 1 \,. \end{aligned}$$

(The diagonal elements follow as well from (10); the off-diagonal elements are complex conjugated w.r.t. each other.)

(iv) In (5) we have

$$\begin{pmatrix} a_- \\ a'_+ \end{pmatrix} = \begin{pmatrix} r \\ t \end{pmatrix}, \qquad \begin{pmatrix} a_+ \\ a'_- \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix};$$

in (6)

$$\begin{pmatrix} a_- \\ a'_+ \end{pmatrix} = \begin{pmatrix} t' \\ r' \end{pmatrix}, \qquad \begin{pmatrix} a_+ \\ a'_- \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

In these cases, equation (8) is satisfied. Hence (8) generally holds true, since every solution can be written as a linear combination of (5) and (6), which amounts to linear combinations of the coefficients. Solving for a_-, a'_+ in (3), we get

$$\begin{aligned} r &= \frac{T_{-+}}{T_{++}} \,, & t' &= \frac{\det T}{T_{++}} \,, \\ t &= \frac{1}{T_{++}} \,, & r' &= -\frac{T_{+-}}{T_{++}} \,. \end{aligned} \tag{11}$$

On the other hand, this also implies

$$\begin{aligned} T_{++} &= \frac{1}{t} \,, & T_{+-} &= -\frac{r'}{t} \,, \\ T_{-+} &= \frac{r}{t} \,, & T_{--} &= \frac{\xi}{t} \end{aligned}$$

where $\xi = tt' - rr'$. In particular, we have $\det T = T_{++}t' = t'/t$.

(v) The transfer matrix clearly is multiplicative:

$$T = T_1T_2 = \frac{1}{t_1t_2}\begin{pmatrix} 1 - r'_1r_2 & -r'_2 - r'_1\xi_2 \\ r_1 + r_2\xi_1 & * \end{pmatrix}.$$

In particular, $\det T = t'_1 t'_2 / t_1 t_2$. By (11), we have for the (non-multiplicative) scattering matrix

$$r = r_1 + \frac{r_2 t_1 t'_1}{1 - r'_1 r_2}\,, \qquad t' = \frac{t'_1 t'_2}{1 - r'_1 r_2}\,,$$
$$t = \frac{t_1 t_2}{1 - r'_1 r_2}\,, \qquad r' = r'_2 + \frac{r'_1 t_2 t'_2}{1 - r'_1 r_2}\,.$$

These results can also be found without the use of the transfer matrix, e.g. for t we have

$$t = t_1 \sum_{n=0}^{\infty} (r_2 r'_1)^n t_2\,,$$

because the particle can be transmitted immediately from the left to the right ($n = 0$), or only after $n = 1, 2, \ldots$ times traveling the way forward and backwards between the scatterers. The sum is a geometric series, thus $(1 - r_2 r'_1)^{-1}$.

(vi) For $A(x) \equiv 0$, (2) has real coefficients, which implies the hint. Hence with (5), also

$$\overline{\psi_1(x)} = \begin{cases} \bar{r} e^{ikx} + e^{-ikx}\,, & (x \leqslant a) \\ \bar{t} e^{-ikx}\,, & (x \geqslant b) \end{cases}$$

is a solution:

$$S \begin{pmatrix} \bar{r} \\ \bar{t} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}\,,$$

i.e. $r\bar{r} + \bar{t}t' = 1$, $t\bar{r} + r'\bar{t} = 0$. Comparing with (7), one finds $t = t'$. S then is symmetric, and $\det T = 1$.