
8 The quantum theory of motion

8A Translation

Answers to discussion questions

- D8A.1** In quantum mechanics, particles are said to have wave characteristics. The fact of the existence of the particle then requires that the wavelengths of the waves representing it be such that the wave does not experience destructive interference upon reflection by a barrier or in its motion around a closed loop. This requirement restricts the wavelength to values $\lambda = 2 / n \times L$, where L is the length of the path and n is a positive integer. Then using the relations $\lambda = h/p$ and $E = p^2 / 2m$, the energy is quantized at $E = n^2 h^2 / 8mL^2$. This derivation applies specifically to the particle in a box, the derivation is similar for the particle on a ring; the same principles apply. (See Section 8C.1).
- D8A.3** The physical origin of tunnelling is related to the probability density of the particle, which according to the Born interpretation is the square of the wavefunction that represents the particle. This interpretation requires that the wavefunction of the system be everywhere continuous, even at barriers. Therefore, if the wavefunction is non zero on one side of a barrier it must be non zero on the other side of the barrier and this implies that the particle has tunneled into the barrier. The transmission probability depends upon the mass of the particle (specifically $m^{1/2}$, through eqns 8A.21): the greater the mass the smaller the probability of tunnelling. Electrons and protons have small masses, molecular groups large masses; therefore, tunnelling effects are more observable in process involving electrons and protons.

Solutions to exercises

- E8A.1(a)** If the wavefunction is an eigenfunction of an operator, the corresponding eigenvalue is the value of corresponding observable [Section 7C.1(b)]. Applying the linear momentum operator $\hat{p} = \frac{\hbar}{i} \frac{d}{dx}$ [7C.3] to the wavefunction yields

$$\hat{p}\psi = \frac{\hbar}{i} \frac{d}{dx} \psi = \frac{\hbar}{i} \frac{d}{dx} e^{ikx} = \hbar k e^{ikx}$$

so the wavefunction is an eigenfunction of the linear momentum; thus, the value of the linear momentum is the eigenvalue

$$\hbar k = 1.0546 \times 10^{-34} \text{ Js} \times 3 \times (10^{-9} \text{ m})^{-1} = \boxed{3 \times 10^{-25} \text{ kg ms}^{-1}}$$

Similarly, applying the kinetic energy operator $\hat{E}_k = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$ [7C.5] to the wavefunction yields

$$\hat{E}_k \psi = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} e^{ikx} = \frac{\hbar^2 k^2}{2m} e^{ikx}$$

so the wavefunction is an eigenfunction of this operator as well; thus, its value is the eigenvalue

$$\frac{\hbar^2 k^2}{2m} = \frac{\{1.0546 \times 10^{-34} \text{ Js} \times 3 \times (10^{-9} \text{ m})^{-1}\}^2}{2 \times 9.11 \times 10^{-31} \text{ kg}} = \boxed{5 \times 10^{-20} \text{ J}}$$

- E8A.2(a)** The wavefunction for the particle is [8A.2 with $B=0$ because the particle is moving toward positive x]

$$\psi_k = \boxed{Ae^{ikx}}$$

The index k is given by the relationship

$$E_k = \frac{\hbar^2 k^2}{2m} = 20 \text{ J}$$

$$\text{so } k = \frac{\sqrt{2mE_k}}{\hbar} = \frac{(2(2.0 \times 10^{-3} \text{ kg})(20 \text{ J}))^{1/2}}{1.0546 \times 10^{-34} \text{ Js}} = \boxed{2.7 \times 10^{33} \text{ m}^{-1}}$$

E8A.3(a) $E = \frac{n^2 h^2}{8m_e L^2}$ [8A.6b]

$$\frac{h^2}{8m_e L^2} = \frac{(6.626 \times 10^{-34} \text{ Js})^2}{(8) \times (9.11 \times 10^{-31} \text{ kg}) \times (1.0 \times 10^{-9} \text{ m})^2} = 6.02 \times 10^{-20} \text{ J}$$

The conversion factors required are

$$1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}; \quad 1 \text{ cm}^{-1} = 1.986 \times 10^{-23} \text{ J}; \quad 1 \text{ eV} = 96.485 \text{ kJ mol}^{-1}$$

$$\begin{aligned} \text{(i) } E_2 - E_1 &= (4-1) \frac{h^2}{8m_e L^2} = \frac{3h^2}{8m_e L^2} = (3) \times (6.02 \times 10^{-20} \text{ J}) \\ &= \boxed{1.81 \times 10^{-19} \text{ J}}, \quad \boxed{1.13 \text{ eV}}, \quad \boxed{9100 \text{ cm}^{-1}}, \quad \boxed{109 \text{ kJ mol}^{-1}} \end{aligned}$$

$$\begin{aligned} \text{(ii) } E_6 - E_5 &= (36-25) \frac{h^2}{8m_e L^2} = \frac{11h^2}{8m_e L^2} = (11) \times (6.02 \times 10^{-20} \text{ J}) \\ &= \boxed{6.6 \times 10^{-19} \text{ J}}, \quad \boxed{4.1 \text{ eV}}, \quad \boxed{33000 \text{ cm}^{-1}}, \quad \boxed{400 \text{ kJ mol}^{-1}} \end{aligned}$$

Comment. The energy level separations increase as n increases.

Question. For what value of n is $E_{n+1} - E_n$ for the system of this exercise equal to the ionization energy of the hydrogen atom, which is 13.6 eV?

E8A.4(a) The wavefunctions are [8A.6a]

$$\psi_n = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right)$$

The required probability is

$$P = \int \psi^* \psi dx = \frac{2}{L} \int \sin^2\left(\frac{n\pi x}{L}\right) dx \approx \frac{2\Delta x}{L} \sin^2\left(\frac{n\pi x}{L}\right)$$

where $\Delta x = 0.02L$ and the function is evaluated at $x = 0.50L$.

$$(i) \text{ For } n=1 \quad P = \left(\frac{2}{L}\right) \times 0.02L \times \sin^2\left(\frac{\pi}{2}\right) = \boxed{0.04}$$

$$(ii) \text{ For } n=2 \quad P = \left(\frac{2}{L}\right) \times 0.02L \times \sin^2 \pi = 0 \quad \text{so } P \approx \boxed{0}$$

E8A.5(a) The wavefunction for a particle in a square-well potential is [8A.6a]

$$\psi_1 = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right)$$

and the momentum operator is [7C.3]

$$\hat{p} = \frac{\hbar}{i} \frac{d}{dx}$$

$$\begin{aligned} \text{so } \langle p \rangle &= \int_0^L \psi_1^* \hat{p} \psi_1 dx = \frac{2\hbar}{iL} \int_0^L \sin\left(\frac{n\pi x}{L}\right) \frac{d}{dx} \sin\left(\frac{n\pi x}{L}\right) dx \\ &= \frac{2\pi\hbar}{iL^2} \int_0^L \sin\left(\frac{n\pi x}{L}\right) \cos\left(\frac{n\pi x}{L}\right) dx = \boxed{0} \text{ for all } n \text{ including } n=1 \end{aligned}$$

$$\hat{p}^2 = -\hbar^2 \frac{d^2}{dx^2}$$

$$\begin{aligned} \langle p^2 \rangle &= -\frac{2\hbar^2}{L} \int_0^L \sin\left(\frac{n\pi x}{L}\right) \frac{d^2}{dx^2} \sin\left(\frac{n\pi x}{L}\right) dx = \left(\frac{2\hbar^2}{L}\right) \times \left(\frac{n\pi}{L}\right)^2 \int_0^L \sin^2 ax dx \left[a = \frac{n\pi}{L} \right] \\ &= \left(\frac{2\hbar^2}{L}\right) \times \left(\frac{n\pi}{L}\right)^2 \left(\frac{1}{2}x - \frac{1}{4a} \sin 2ax \right) \Big|_0^L = \left(\frac{2\hbar^2}{L}\right) \times \left(\frac{n\pi}{L}\right)^2 \times \left(\frac{L}{2}\right) = \frac{n^2 \hbar^2}{4L^2} \end{aligned}$$

$$\text{So for } n=1: \langle p^2 \rangle = \boxed{\frac{\hbar^2}{4L^2}}$$

Comment. The expectation value of \hat{p} is zero because on average the particle moves to the left as often as the right.

E8A.6(a) The wavefunction is

$$\psi_n = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right) \quad [8A.6a]$$

$$\text{Hence } \langle x \rangle = \int \psi^* x \psi dx = \frac{2}{L} \int_0^L x \sin^2\left(\frac{n\pi x}{L}\right) dx$$

Use Integral T.11 from the *Resource section*

$$\int x \sin^2 ax dx = \frac{x^2}{4} - \frac{x \sin 2ax}{4a} - \frac{\cos 2ax}{8a^2}$$

$$\text{so } \langle x \rangle = \frac{2}{L} \left[\frac{x^2}{4} - \frac{Lx}{4n\pi} \sin\left(\frac{2n\pi x}{L}\right) - \frac{L^2}{8(n\pi)^2} \cos\left(\frac{2n\pi x}{L}\right) \right]_0^L = \left[\frac{L}{2} \right] \text{ for all } n.$$

$$\langle x^2 \rangle = \frac{2}{L} \int_0^L x^2 \sin^2\left(\frac{n\pi x}{L}\right) dx$$

Use Integral T.12 from the *Resource section*

$$\int x^2 \sin^2 ax dx = \frac{x^3}{6} - \left(\frac{x^2}{4a} - \frac{1}{8a^3}\right) \sin 2ax - \frac{x \cos 2ax}{4a^2}$$

$$\begin{aligned} \text{so } \langle x^2 \rangle &= \frac{2}{L} \left[\frac{x^3}{6} - \left(\frac{Lx^2}{4n\pi} - \frac{L^3}{(2n\pi)^3}\right) \sin\left(\frac{2n\pi x}{L}\right) - \frac{L^2 x}{(2n\pi)^2} \cos\left(\frac{2n\pi x}{L}\right) \right]_0^L \\ &= \frac{2}{L} \left(\frac{L^3}{6} - \frac{L^3}{(2n\pi)^2} \right) = L^2 \left(\frac{1}{3} - \frac{1}{2n^2\pi^2} \right) \end{aligned}$$

$$\text{For } n=1, \langle x^2 \rangle = L^2 \left(\frac{1}{3} - \frac{1}{2\pi^2} \right)$$

E8A.7(a) The zero-point energy is the ground-state energy, that is, with $n=1$:

$$E = \frac{n^2 h^2}{8m_e L^2} [8A.6b] = \frac{h^2}{8m_e L^2}$$

Set this equal to the rest energy $m_e c^2$ and solve for L :

$$m_e c^2 = \frac{h^2}{8m_e L^2} \quad \text{so } L = \left[\frac{h}{8^{1/2} m_e c} \right] = \frac{\lambda_C}{8^{1/2}}$$

In absolute units, the length is

$$L = \frac{6.63 \times 10^{-34} \text{ J s}}{8^{1/2} \times (9.11 \times 10^{-31} \text{ kg}) \times (3.00 \times 10^8 \text{ m s}^{-1})} = 8.58 \times 10^{-13} \text{ m} = 0.858 \text{ pm}$$

In terms of the Compton wavelength of an electron, $\lambda_C = \frac{h}{m_e c}$, $L = \frac{\lambda_C}{2\sqrt{2}}$.

$$\text{E8A.8(a)} \quad \psi_3 = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{3\pi x}{L}\right) \quad [8A.6a]$$

$$P(x) \propto \psi_3^2 \propto \sin^2\left(\frac{3\pi x}{L}\right)$$

The maxima and minima in $P(x)$ correspond to $\frac{dP(x)}{dx} = 0$.

$$\frac{dP(x)}{dx} \propto \sin\left(\frac{3\pi x}{L}\right) \cos\left(\frac{3\pi x}{L}\right) \propto \sin\left(\frac{6\pi x}{L}\right) \quad [2\sin\alpha \cos\alpha = \sin 2\alpha]$$

$\sin\theta = 0$ when $\theta = \left(\frac{6\pi x}{L}\right) = n'\pi$, $n' = 0, 1, 2, \dots$, which corresponds to $x = \frac{n'L}{6}$, $n' \leq 6$.

$n' = 0, 2, 4$, and 6 correspond to minima in P , leaving $n' = 1, 3$, and 5 for the maxima, that is

$$x = \left[\frac{L}{6}, \frac{L}{2}, \text{ and } \frac{5L}{6} \right]$$

Comment. Maxima in ψ^2 correspond to maxima *and* minima in ψ itself, so one can also solve this exercise by finding all points where $\frac{d\psi}{dx} = 0$.

E8A.9(a) In the original box [8A.6b]

$$E_1 = \frac{n^2 h^2}{8mL^2}$$

In the longer box

$$E_2 = \frac{n^2 h^2}{8m(1.1L)^2}$$

$$\text{So} \quad \Delta E = \frac{n^2 h^2}{8mL^2} \left(\frac{1}{1.1^2} - 1 \right)$$

and the relative change is

$$\frac{\Delta E}{E_1} = \frac{1}{1.1^2} - 1 = -0.174 = \boxed{-17.4\%}$$

E8A.10(a) The energy is [8A.6b]

$$E_n = \frac{n^2 h^2}{8mL^2}$$

so the difference between neighbouring levels is

$$\Delta E_n = E_{n+1} - E_n = \frac{\{(n+1)^2 - n^2\}h^2}{8mL^2} = \frac{(2n+1)h^2}{8mL^2}$$

Set this difference equal to the thermal energy $kT/2$ and solve for n :

$$\frac{(2n+1)h^2}{8mL^2} = \frac{kT}{2},$$

$$\text{so } n = \frac{2kTmL^2}{h^2} - \frac{1}{2}$$

E8A.11(a) The energy levels are given by [8A.15b]

$$E_{n_1, n_2} = \left(\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} \right) \frac{h^2}{8m} = \left(\frac{n_1^2}{1} + \frac{n_2^2}{4} \right) \frac{h^2}{8mL^2}$$

$$E_{2,2} = \left(\frac{2^2}{1} + \frac{2^2}{4} \right) \frac{h^2}{8mL^2} = \frac{5h^2}{8mL^2}$$

We are looking for another state that has the same energy. By inspection we note that the first term in parentheses in $E_{2,2}$ works out to be 4 and the second 1; we can arrange for those values to be reversed:

$$E_{1,4} = \left(\frac{1^2}{1} + \frac{4^2}{4} \right) \frac{h^2}{8mL^2} = \frac{5h^2}{8mL^2}$$

So in this box, the state $\boxed{n_1=1, n_2=4}$ is degenerate to the state $n_1=2, n_2=2$. The question notes that degeneracy frequently accompanies symmetry, and suggests that one might be surprised to find degeneracy in a box with unequal lengths. Symmetry is a matter of degree. This box is less symmetric than a square box, but it is more symmetric than boxes whose sides have a non-integer or irrational ratio. Every state of a square box except those with $n_1=n_2$ is degenerate (with the state that has n_1 and n_2 reversed). Only a few states in this box are degenerate. In this system, a state (n_1, n_2) is degenerate with a state $(n_2/2, 2n_1)$ as long as the latter state (a) exists (*i.e.*, $n_2/2$ must be an integer) and (b) is distinct from (n_1, n_2) . A box with incommensurable sides, say, L and $2^{1/2}L$, would have no degenerate levels.

E8A.12(a) $E_{n_1, n_2, n_3} = \frac{(n_1^2 + n_2^2 + n_3^2)h^2}{8m_e L^2}$ [8A.16b]

$$E_{1,1,1} = \frac{3h^2}{8mL^2}, \quad 3E_{1,1,1} = \frac{9h^2}{8mL^2}$$

Hence, we require the values of n_1 , n_2 , and n_3 that make

$$n_1^2 + n_2^2 + n_3^2 = 9$$

Therefore, $(n_1, n_2, n_3) = (1, 2, 2), (2, 1, 2),$ and $(2, 2, 1)$ and the degeneracy is $\boxed{3}$.

E8A.13(a) The transmission probability [8A.23a] depends on the energy of the tunneling particle relative to the barrier height ($\epsilon = E/V = 1.5 \text{ eV}/(2.0 \text{ eV}) = 0.75$), on the width of the barrier ($L = 100 \text{ pm}$), and on the decay parameter of the wavefunction inside the barrier (κ), where [8A.20]

$$\begin{aligned} \kappa &= \frac{\{2m(V-E)\}^{1/2}}{\hbar} = \frac{\{2 \times 9.11 \times 10^{-31} \text{ kg} \times (2.0 - 1.5) \text{ eV} \times 1.602 \times 10^{-19} \text{ J eV}^{-1}\}^{1/2}}{1.0546 \times 10^{-34} \text{ Js}} \\ &= 3.6 \times 10^9 \text{ m}^{-1} \end{aligned}$$

We note that $\kappa L = 3.6 \times 10^9 \text{ m}^{-1} \times 100 \times 10^{-12} \text{ m} = 0.36$ is not large compared to 1, so we must use eqn 8A.23a for the transmission probability.

$$T = \left\{ 1 + \frac{(e^{\kappa L} - e^{-\kappa L})^2}{16\varepsilon(1-\varepsilon)} \right\}^{-1} = \left\{ 1 + \frac{(e^{0.36} - e^{-0.36})^2}{16 \times 0.75 \times (1-0.75)} \right\}^{-1} = \boxed{0.8}$$

Solutions to problems

P8A.1 $E = \frac{n^2 h^2}{8mL^2}$ [8A.6b], $E_2 - E_1 = \frac{3h^2}{8mL^2}$

For O_2 , $m = 32.00 \times (1.6605 \times 10^{-27} \text{ kg}) = 5.314 \times 10^{-26} \text{ kg}$,

so $E_2 - E_1 = \frac{(3) \times (6.626 \times 10^{-34} \text{ Js})^2}{(8) \times (5.314 \times 10^{-26} \text{ kg}) \times (5.0 \times 10^{-2} \text{ m})^2} = \boxed{1.24 \times 10^{-39} \text{ J}}$

We set $E = \frac{n^2 h^2}{8mL^2} = \frac{kT}{2}$ and solve for n :

$$\begin{aligned} n &= \frac{2L(kTm)^{1/2}}{h} \\ &= \frac{2 \times (5.0 \times 10^{-2} \text{ m}) \times \{(1.381 \times 10^{-23} \text{ JK}^{-1}) \times (300 \text{ K}) \times 5.314 \times 10^{-26} \text{ kg}\}^{1/2}}{6.626 \times 10^{-34} \text{ Js}} \\ &= \boxed{2.2 \times 10^9} \end{aligned}$$

At this level,

$$E_n - E_{n-1} = \{n^2 - (n-1)^2\} \times \frac{h^2}{8mL^2} = (2n-1) \times \frac{h^2}{8mL^2} \approx (2n) \times \frac{h^2}{8mL^2}$$

From above $\frac{h^2}{8mL^2} = \frac{E_2 - E_1}{3} = 4.13 \times 10^{-40} \text{ J}$,

so $E_n - E_{n-1} = 2 \times (2.2 \times 10^9) \times (4.13 \times 10^{-40} \text{ J}) \approx \boxed{1.8 \times 10^{-30} \text{ J}}$ [or $1.1 \mu\text{J mol}^{-1}$]

P8A.3 (a) Suppose that a particle moves classically at the constant speed v . It starts at $x=0$ at $t=0$ and at $t=\tau$ is at position $x=L$. $v = \frac{L}{\tau}$ and $x=vt$.

$$\begin{aligned} \langle x \rangle &= \frac{1}{\tau} \int_{t=0}^{\tau} x \, dt = \frac{1}{\tau} \int_{t=0}^{\tau} vt \, dt = \frac{v}{\tau} \int_{t=0}^{\tau} t \, dt = \frac{v}{2\tau} t^2 \Big|_{t=0}^{\tau} \\ &= \frac{v\tau^2}{2\tau} = \frac{v\tau}{2} = \boxed{\frac{L}{2}} \end{aligned}$$

$$\langle x^2 \rangle = \frac{1}{\tau} \int_{t=0}^{\tau} x^2 \, dt = \frac{v^2}{\tau} \int_{t=0}^{\tau} t^2 \, dt = \frac{v^2}{3\tau} t^3 \Big|_{t=0}^{\tau} = \frac{(v\tau)^2}{3} = \frac{L^2}{3}$$

so $\langle x^2 \rangle^{1/2} = \boxed{\frac{L}{3^{1/2}}}$

$$(b) \psi_n = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right) \text{ for } 0 \leq x \leq L \text{ [8A.7a]}$$

$$\begin{aligned} \langle x \rangle_n &= \int_{x=0}^L \psi_n^* x \psi_n dx = \frac{2}{L} \int_0^L x \sin^2\left(\frac{n\pi x}{L}\right) dx \\ &= \frac{2}{L} \left[\frac{x^2}{4} - \frac{x \sin\left(\frac{2n\pi x}{L}\right)}{4(n\pi/L)} - \frac{\cos\left(\frac{2n\pi x}{L}\right)}{8(n\pi/L)^2} \right] \Bigg|_{x=0}^{x=L} = \frac{2}{L} \left(\frac{L^2}{4} \right) = \boxed{\frac{L}{2}} \end{aligned}$$

This agrees with the classical result for all values of n .

$$\begin{aligned} \langle x^2 \rangle_n &= \int_{x=0}^L \psi_n^* x^2 \psi_n dx = \frac{2}{L} \int_{x=0}^L x^2 \sin^2\left(\frac{n\pi x}{L}\right) dx \\ &= \frac{2}{L} \left[\frac{x^3}{6} - \left(\frac{x^2}{4(n\pi/L)} - \frac{1}{8(n\pi/L)^3} \right) \sin\left(\frac{2n\pi x}{L}\right) - \frac{x \cos\left(\frac{2n\pi x}{L}\right)}{8(n\pi/L)^2} \right] \Bigg|_{x=0}^{x=L} \\ &= \frac{2}{L} \left(\frac{L^3}{6} - \frac{L}{8(n\pi/L)^2} \right) = \frac{L^2}{3} - \frac{1}{4(n\pi/L)^2} \end{aligned}$$

$$\text{so } \langle x^2 \rangle_n^{1/2} = \boxed{\left(\frac{L^2}{3} - \frac{1}{4(n\pi/L)^2} \right)^{1/2}}$$

This agrees with the classical result in the limit of large quantum numbers:

$$\lim_{n \rightarrow \infty} \langle x^2 \rangle_n^{1/2} = \frac{L}{3^{1/2}}$$

P8A.5

The rate of tunnelling is proportional to the transmission probability, so a ratio of tunnelling rates is equal to the corresponding ratio of transmission probabilities (given in eqn 8A.23a). The desired factor is T_1/T_2 , where the subscripts denote the tunnelling distances in nanometres:

$$\frac{T_1}{T_2} = \frac{1 + \frac{(e^{\kappa L_2} - e^{-\kappa L_2})^2}{16\varepsilon(1-\varepsilon)}}{1 + \frac{(e^{\kappa L_1} - e^{-\kappa L_1})^2}{16\varepsilon(1-\varepsilon)}}$$

$$\text{If } \frac{(e^{\kappa L_2} - e^{-\kappa L_2})^2}{16\varepsilon(1-\varepsilon)} \gg 1,$$

$$\text{then } \frac{T_1}{T_2} \approx \frac{(e^{\kappa L_2} - e^{-\kappa L_2})^2}{(e^{\kappa L_1} - e^{-\kappa L_1})^2} \approx e^{2\kappa(L_2 - L_1)} = e^{2(7/\text{nm})(2.0 - 1.0)\text{nm}} = \boxed{1.2 \times 10^6}.$$

That is, the tunnelling rate increases about a million-fold. Note: if the first approximation does not hold, we need more information, namely $\varepsilon = E/V$. If the first approximation is valid, then the second is also likely to be valid, namely that the negative exponential is negligible compared to the positive one.

- P8A.7 (a) The wavefunctions in each region (see Fig. 8A.1(a)) are (eqns 8A.18, 8A.20, and 8A.21):

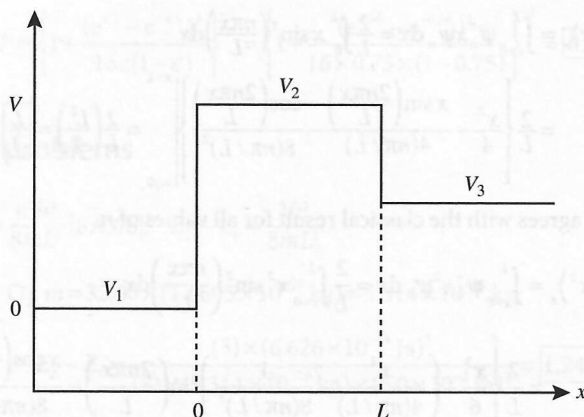


Figure 8A.1(a)

$$\psi_1(x) = e^{ik_1x} + B_1e^{-ik_1x}$$

$$\psi_2(x) = A_2e^{k_2x} + B_2e^{-k_2x}$$

$$\psi_3(x) = A_3e^{ik_3x}$$

With the above choice of $A_1 = 1$ the transmission probability is simply $T = |A_3|^2$. The wavefunction coefficients are determined by the criteria that both the wavefunctions and their first derivatives with respect to x be continuous at potential boundaries

$$\psi_1(0) = \psi_2(0) \quad \text{and} \quad \psi_2(L) = \psi_3(L)$$

$$\frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx} \quad \text{and} \quad \frac{d\psi_2(L)}{dx} = \frac{d\psi_3(L)}{dx}$$

These criteria establish the algebraic relationships:

$$1 + B_1 - A_2 - B_2 = 0$$

$$(-ik_1 - k_2)A_2 + (-ik_1 + k_2)B_2 + 2ik_1 = 0$$

$$A_2e^{k_2L} + B_2e^{-k_2L} - A_3e^{ik_3L} = 0$$

$$A_2k_2e^{k_2L} - B_2k_2e^{-k_2L} - iA_3k_3e^{ik_3L} = 0$$

Solving the simultaneous equations for A_3 gives

$$A_3 = \frac{4k_1k_2e^{ik_3L}}{(ia+b)e^{k_2L} - (ia-b)e^{-k_2L}}$$

where $a = k_2^2 - k_1k_3$ and $b = k_1k_2 + k_2k_3$

Since $\sinh(z) = (e^z - e^{-z})/2$ or $e^z = 2 \sinh(z) + e^{-z}$, substitute $e^{k_2 L} = 2 \sinh(k_2 L) + e^{-k_2 L}$ giving

$$A_3 = \frac{2k_1 k_2 e^{ik_3 L}}{(ia + b) \sinh(k_2 L) + b e^{-k_2 L}}$$

the transmission coefficient is

$$T = |A_3|^2 = A_3 \times A_3^* = \frac{4k_1^2 k_2^2}{(a^2 + b^2) \sinh^2(k_2 L) + b^2}$$

where $a^2 + b^2 = (k_1^2 + k_2^2)(k_2^2 + k_3^2)$ and $b^2 = k_2^2(k_1 + k_3)^2$

(b) In the special case for which $V_1 = V_3 = 0$, eqns 8A.18 and 8A.21 require that $k_1 = k_3$. Additionally,

$$\left(\frac{k_1}{k_2}\right)^2 = \frac{E}{V_2 - E} = \frac{\varepsilon}{1 - \varepsilon} \text{ where } \varepsilon = E/V_2.$$

$$a^2 + b^2 = (k_1^2 + k_2^2)^2 = k_2^4 \left[1 + \left(\frac{k_1}{k_2}\right)^2\right]^2$$

$$b^2 = 4k_1^2 k_2^2$$

$$\frac{a^2 + b^2}{b^2} = \frac{k_2^2 \left[1 + \left(\frac{k_1}{k_2}\right)^2\right]^2}{4k_1^2}$$

$$= \frac{1}{4\varepsilon(1 - \varepsilon)}$$

$$T = \frac{b^2}{b^2 + (a^2 + b^2) \sinh^2(k_2 L)} = \frac{1}{1 + \left(\frac{a^2 + b^2}{b^2}\right) \sinh^2(k_2 L)}$$

$$= \left[1 + \frac{\sinh^2(k_2 L)}{4\varepsilon(1 - \varepsilon)}\right]^{-1}$$

$$= \left[1 + \frac{(e^{k_2 L} - e^{-k_2 L})^2}{16\varepsilon(1 - \varepsilon)}\right]^{-1}$$

This proves eqn 8A.23a where $V_1 = V_3 = 0$

In the limit of a high and wide barrier, $k_2 L \gg 1$. This implies both that $e^{-k_2 L}$ is negligibly small compared to $e^{k_2 L}$ and that 1 is negligibly small compared to $e^{2k_2 L} / \{16\varepsilon(1 - \varepsilon)\}$. The previous equation simplifies to [8A.23b]

$$T = 16\varepsilon(1 - \varepsilon)e^{-2k_2 L}$$

(c) The specified graph is shown in Fig. 8A.1(b).

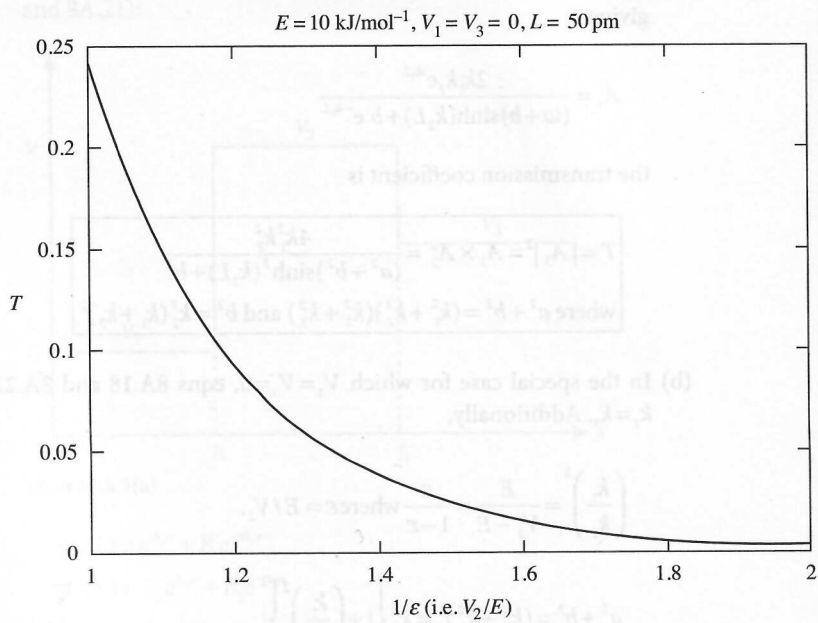


Figure 8A.1(b)