

**20** 6. Show that as  $U_0 \rightarrow 0$ , the transmission coefficient  $T(E) \rightarrow 1$  for both cases  $E > U_0$  and  $E < U_0$ .

**Case 1:**  $E > U_0$

The transmission coefficient is given by:

$$T(E) = \frac{4k_1^2 k_2^2}{4k_1^2 k_2^2 \cos^2(k_2 a) + (k_1^2 - k_2^2)^2 \sin^2(k_2 a)}$$

where

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}}, \quad k_2 = \sqrt{\frac{2m(E - U_0)}{\hbar^2}}$$

As  $U_0 \rightarrow 0$ , so  $k_2 \rightarrow k_1$ , and thus:

$$k_1^2 - k_2^2 \rightarrow 0$$

This simplifies the expression to:

$$T(E) \rightarrow \frac{4k_1^4}{4k_1^4} = 1$$

**Case 2:**  $E < U_0$

The transmission coefficient is:

$$T(E) = \frac{4k_1^2 k_2^2}{4k_1^2 k_2^2 \cosh^2(k_2 a) + (k_1^2 + k_2^2)^2 \sinh^2(k_2 a)}$$

where

$$k_2 = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$$

As  $U_0 \rightarrow 0$ ,  $k_2 \rightarrow 0$ . Taylor expansions for small arguments:

$$\cosh(k_2 a) \approx 1 + \frac{(k_2 a)^2}{2}, \quad \sinh(k_2 a) \approx k_2 a$$

Substituting into the denominator:

$$\cosh^2(k_2 a) \approx 1 + (k_2 a)^2, \quad \sinh^2(k_2 a) \approx (k_2 a)^2$$

Thus, the denominator becomes:

$$4k_1^2 k_2^2 (1 + (k_2 a)^2) + (k_1^2 + k_2^2)^2 (k_2 a)^2$$

As  $k_2 \rightarrow 0$ , the terms involving  $(k_2 a)^2$  vanish, and it simplifies to:

$$4k_1^2 k_2^2$$

So:

$$T(E) \rightarrow \frac{4k_1^2 k_2^2}{4k_1^2 k_2^2} = 1$$

20

**8. Show that the probability current density (or wavefunction) inside the walls (areas 1 and 3) of an infinite potential well should be zero, and explain why.**

The probability current density  $J(x, t)$  is defined as:

$$J(x, t) = \frac{\hbar}{2mi} \left( \psi^*(x, t) \frac{\partial \psi(x, t)}{\partial x} - \psi(x, t) \frac{\partial \psi^*(x, t)}{\partial x} \right)$$

where:

- $\hbar$  is the reduced Planck constant,
- $m$  is the mass of the particle,
- $\psi(x, t)$  is the wavefunction.

In regions outside the well, the potential  $U(x)$  is infinite:

$$U(x) = \infty \quad \text{for } x \leq 0 \quad \text{or } x \geq L$$

the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + U(x) \psi(x) = E \psi(x)$$

Substituting  $U(x) = \infty$  leads to:

$$\infty \times \psi(x) = E\psi(x) + (\text{finite terms})$$

For the equation to remain finite on both sides, the only solution is:

$$\psi(x) = 0$$

If  $\psi(x) \neq 0$ , the left side would be infinite, which is impossible. Therefore the probability of finding the particle there is zero.

Since  $\psi(x) = 0$  and  $\frac{\partial\psi}{\partial x} = 0$ , substituting into the expression  $J(x, t)$  gives:

$$J(x, t) = 0$$

**15 18. Should the wave function inside the walls of a finite potential well be a complex number or a real number? What is your opinion, and why?**

The general solution in this region is:

$$\psi(x) = Ae^{\kappa x} + Be^{-\kappa x}$$

where

$$\kappa = \sqrt{\frac{2m(U - E)}{\hbar^2}}$$

is a positive real constant since  $U > E$  (bound state). Since both  $e^{\kappa x}$  and  $e^{-\kappa x}$  are real functions, and the coefficients  $A$  and  $B$  can be taken to be real as well, the wave function  $\psi(x)$  itself can be real. Complex exponentials are needed when  $U < E$  and the solution is oscillatory.

**20 28. How can we calculate the energy of a harmonic oscillator at a non-zero temperature?**

**Note:** Thermal motion is fully chaotic and can be described by a random force acting on an oscillating point mass. Ideas from the calculation of heat capacity in a 1D crystal lattice may be helpful.

The average energy  $\bar{E}$  of a harmonic oscillator is:

$$\bar{E} = \hbar\omega \left( \frac{1}{e^{\hbar\omega/kT} - 1} \right)$$

where:

- $\hbar$  is the reduced Planck constant,
- $\omega$  is the angular frequency of the oscillator,
- $k$  is the Boltzmann constant,
- $T$  is the absolute temperature.

This result comes from the Bose-Einstein distribution, which gives the average occupation number  $\bar{n}$  of the energy levels (for phonons and protons):

$$\bar{n} = \frac{1}{e^{\hbar\omega/kT} - 1}$$

The total thermal energy is then obtained by integrating over all vibrational modes. In 1D crystal models, this leads to:

$$\bar{E}_{\text{tot}} = \frac{2N}{\pi} \int_0^{\omega_0} \frac{\hbar\omega}{\sqrt{\omega_0^2 - \omega^2}} \frac{1}{e^{\hbar\omega/kT} - 1} d\omega$$

where:

- $N$  is the total number of atoms,
- $\omega_0$  is the maximum vibrational frequency  $\omega_0 = \sqrt{\frac{4g}{m}}$

20

**31 Show that the functions  $\omega(q) = \omega_0 \cdot \left| \sin\left(\frac{qa}{2}\right) \right|$  and  $\omega\left(q + \frac{2\pi}{a}\right)$  describe the same harmonic wave  $u_{k,q}(t) = A_q \cdot e^{i(\omega(q)t + qak)}$ . (By other words, show that  $u_{k,q}(t) = u_{k,q+\frac{2\pi}{a}}(t)$ .)**

We are asked to show that:

$$u_{k,q}(t) = u_{k,q+\frac{2\pi}{a}}(t)$$

where:

$$u_{k,q}(t) = A_q e^{i(\omega(q)t + qak)}$$

and

$$\omega(q) = \omega_0 \left| \sin\left(\frac{qa}{2}\right) \right|$$

Substituting  $q + \frac{2\pi}{a}$  instead of  $q$ , we get:

$$u_{k, q + \frac{2\pi}{a}}(t) = A_{q + \frac{2\pi}{a}} e^{i(\omega(q + \frac{2\pi}{a})t + (q + \frac{2\pi}{a})ak)}$$

Expanding the phase:

$$= A_{q + \frac{2\pi}{a}} e^{i(\omega(q + \frac{2\pi}{a})t + qak + 2\pi k)}$$

Since  $e^{i2\pi k} = 1$  for any integer  $k$ , we simplify:

$$= A_{q + \frac{2\pi}{a}} e^{i(\omega(q + \frac{2\pi}{a})t + qak)}$$

Comparing  $\omega(q)$  and  $\omega(q + \frac{2\pi}{a})$

$$\omega\left(q + \frac{2\pi}{a}\right) = \omega_0 \left| \sin\left(\frac{(q + \frac{2\pi}{a})a}{2}\right) \right| = \omega_0 \left| \sin\left(\frac{qa}{2} + \pi\right) \right|$$

Using:

$$\sin(x + \pi) = -\sin(x)$$

Thus:

$$\sin\left(\frac{qa}{2} + \pi\right) = -\sin\left(\frac{qa}{2}\right)$$

Taking the absolute value:

$$\left| \sin\left(\frac{qa}{2} + \pi\right) \right| = \left| -\sin\left(\frac{qa}{2}\right) \right| = \left| \sin\left(\frac{qa}{2}\right) \right|$$

Thus:

$$\omega\left(q + \frac{2\pi}{a}\right) = \omega(q)$$

substituting back, we have:

$$u_{k, q + \frac{2\pi}{a}}(t) = A_{q + \frac{2\pi}{a}} e^{i(\omega(q)t + qak)}$$

If we choose:

$$A_{q + \frac{2\pi}{a}} = A_q$$

then:

$$u_{k,q+\frac{2\pi}{a}}(t) = u_{k,q}(t)$$