

- 20 1. How is looks like Schrodinger equation for tunnel effect (topic 4.3) for regions I,II, and III ? Derive equations.

The time-independent Schrödinger equation in one dimension is

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

For a rectangular barrier of height  $V_0$  extending from  $x = 0$  to  $x = a$ , we split space into three regions:

**Region I:**  $x < 0$ ,  $V(x) = 0$

$$-\frac{\hbar^2}{2m} \psi''(x) = E \psi(x) \implies \psi''(x) + k^2 \psi(x) = 0, \quad k = \frac{\sqrt{2mE}}{\hbar}.$$

General solution:

$$\psi_I(x) = A e^{ikx} + B e^{-ikx}.$$

**Region II:**  $0 \leq x \leq a$ ,  $V(x) = V_0$

$$-\frac{\hbar^2}{2m} \psi''(x) + V_0 \psi(x) = E \psi(x) \implies \psi''(x) + q^2 \psi(x) = 0, \quad q^2 = \frac{2m(E - V_0)}{\hbar^2}.$$

For the tunneling case  $E < V_0$ , define  $\kappa = \sqrt{2m(V_0 - E)}/\hbar$ . Then the equation becomes

$$\psi''(x) - \kappa^2 \psi(x) = 0,$$

with solution

$$\psi_{II}(x) = C e^{\kappa x} + D e^{-\kappa x}.$$

**Region III:**  $x > a$ ,  $V(x) = 0$  Again

$$\psi''(x) + k^2 \psi(x) = 0, \quad k = \frac{\sqrt{2mE}}{\hbar}.$$

If we assume only a transmitted wave to the right,

$$\psi_{III}(x) = F e^{ikx}.$$

**Continuity conditions at  $x = 0$  and  $x = a$ :**

$$\begin{aligned}\psi_I(0) &= \psi_{II}(0) : & A + B &= C + D, \\ \psi'_I(0) &= \psi'_{II}(0) : & ik(A - B) &= \kappa(C - D), \\ \psi_{II}(a) &= \psi_{III}(a) : & Ce^{\kappa a} + De^{-\kappa a} &= Fe^{ika}, \\ \psi'_{II}(a) &= \psi'_{III}(a) : & \kappa(Ce^{\kappa a} - De^{-\kappa a}) &= ikFe^{ika}.\end{aligned}$$

**Solving for  $B$  and  $F$  (with  $A = 1$  for convenience) gives**

$$B = \frac{(k^2 + \kappa^2) \sinh(\kappa a)}{-2ik\kappa \cosh(\kappa a) + (k^2 - \kappa^2) \sinh(\kappa a)}, F = \frac{2ik\kappa e^{-ika}}{2ik\kappa \cosh(\kappa a) + (k^2 - \kappa^2) \sinh(\kappa a)}$$

Since  $F \neq 0$ , there is a nonzero transmitted amplitude—i.e. particles have a finite probability to “tunnel through” the barrier.

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**11. Why the solution for quantum number  $n = 0$  must be ignored? Give a physical justification**

The wave functions are

$$\psi_n(x) = A \sin(n\pi x/L),$$

with corresponding energies

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2}.$$

Here  $n$  is a positive integer.

If we set  $n = 0$ , then

$$\psi_0(x) = A \sin(0) = 0 \quad \text{everywhere.}$$

That means the wave function is identically zero, so the probability density  $|\psi_0(x)|^2$  is zero everywhere. There is no chance of finding the particle anywhere.

**Physical justification:**

- A wave function must be normalizable and nontrivial so that  $\int |\psi|^2 dx = 1$ .

- The  $n = 0$  solution has  $\int 0 dx = 0$ , so it cannot be normalized to unity.
- It carries no probability and hence does not represent a real physical state.

Therefore, we discard the  $n = 0$  solution and start with  $n = 1, 2, 3, \dots$ , each of which gives a valid, nonzero wavefunction and a real energy.

**10 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, why?**

In quantum mechanics the most general wave function  $\Psi(x, t)$  is a complex-valued function. However, when we solve the time-independent Schrödinger equation for bound states in a finite potential well, we often write

$$\Psi(x, t) = \psi(x) e^{-iEt/\hbar},$$

where the spatial part  $\psi(x)$  satisfies

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

Since  $V(x)$  is real, this ordinary differential equation has real coefficients. Consequently:

- Any complex solution  $\psi(x)$  can be multiplied by a global phase  $e^{i\theta}$  without changing physical predictions.
- We are free to choose that global phase so that  $\psi(x)$  is *real* everywhere inside and outside the well.

**Physical Opinion:** Although the full wave function  $\Psi(x, t)$  must be complex (to carry time dependence and relative phases), the *spatial* bound-state functions  $\psi(x)$  can—and usually are—chosen real. This choice simplifies matching boundary conditions at the walls ( $\psi$  and  $\psi'$  continuous) without losing any physics, because:

1. The real and imaginary parts of any solution each satisfy the same Schrödinger equation.

2. A real  $\psi(x)$  already carries all information about the probability density  $|\psi(x)|^2$ .
3. There is no net probability current for a stationary bound state, so no phase gradient is needed in  $\psi(x)$ .

In summary, fundamentally the quantum state is complex, but for bound-state eigenfunctions of a real potential one usually picks the spatial part real for simplicity and clarity.

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**22. Calculate the mean value of the momentum  $p_x$  for the quantum harmonic oscillator. Use tabular integrals from lectures as needed. Compare your result with the corresponding mean momentum for the classical harmonic oscillator.**

The stationary eigenfunctions of the one-dimensional harmonic oscillator are

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left( \frac{m\omega}{\pi \hbar} \right)^{1/4} H_n \left( \sqrt{\frac{m\omega}{\hbar}} x \right) e^{-\frac{m\omega x^2}{2\hbar}},$$

with energy  $E_n = \hbar\omega (n + \frac{1}{2})$ . The momentum operator is

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

We wish to compute

$$\langle p_x \rangle_n = \int_{-\infty}^{+\infty} \psi_n^*(x) \left( -i\hbar \frac{d}{dx} \right) \psi_n(x) dx.$$

1. Notice that for each  $n$ ,  $\psi_n(x)$  is either an even function (if  $n$  even) or an odd function (if  $n$  odd). Hence

$$\psi_n^*(x) \frac{d\psi_n(x)}{dx}$$

is an odd function of  $x$ .

2. The integral of any odd function over the symmetric interval  $(-\infty, +\infty)$  vanishes:

$$\int_{-\infty}^{+\infty} [\text{odd}(x)] dx = 0.$$

3. Therefore

$$\langle p_x \rangle_n = -i\hbar \int_{-\infty}^{+\infty} \psi_n^*(x) \frac{d\psi_n(x)}{dx} dx = 0.$$

For a classical oscillator of mass  $m$ , angular frequency  $\omega$ , and amplitude  $A$ , the position and momentum are

$$x(t) = A \cos(\omega t + \phi), \quad p(t) = m \dot{x}(t) = -m\omega A \sin(\omega t + \phi).$$

The time-average of  $p(t)$  over one period  $T = 2\pi/\omega$  is

$$\bar{p} = \frac{1}{T} \int_0^T p(t) dt = -\frac{m\omega A}{T} \int_0^T \sin(\omega t + \phi) dt = 0.$$

Both in the quantum case (for any energy level  $n$ ) and in the classical case, the average (mean) momentum over a full cycle vanishes:

$$\boxed{\langle p_x \rangle_n = 0, \quad \bar{p} = 0.}$$

This reflects the symmetry of the motion: there is no net drift in either direction over one full oscillation.

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**37. Can you show that (for a 1D crystal) the phase and group velocities of harmonic waves become equal in the limit of very long wavelengths ( $\lambda \rightarrow \infty$ )?**

Consider a one-dimensional monatomic crystal of atoms of mass  $M$  connected by springs of constant  $C$ , with lattice constant  $a$ . The dispersion relation for small oscillations is

$$\omega(k) = 2\sqrt{\frac{C}{M}} \left| \sin\left(\frac{ka}{2}\right) \right|.$$

The phase velocity is

$$v_{\text{ph}}(k) = \frac{\omega(k)}{k} = \frac{2}{k} \sqrt{\frac{C}{M}} \left| \sin\left(\frac{ka}{2}\right) \right|,$$

and the group velocity is

$$v_{\text{g}}(k) = \frac{d\omega}{dk} = 2\sqrt{\frac{C}{M}} \frac{d}{dk} \left| \sin\left(\frac{ka}{2}\right) \right| = a\sqrt{\frac{C}{M}} \cos\left(\frac{ka}{2}\right).$$

In the long-wavelength limit  $k \rightarrow 0$  (so  $\lambda = 2\pi/k \rightarrow \infty$ ), we use the small-angle approximations

$$\sin\left(\frac{ka}{2}\right) \approx \frac{ka}{2}, \quad \cos\left(\frac{ka}{2}\right) \approx 1.$$

Substituting into the velocities gives

$$v_{\text{ph}}(k) \approx \frac{2}{k} \sqrt{\frac{C}{M}} \frac{ka}{2} = a \sqrt{\frac{C}{M}},$$

$$v_{\text{g}}(k) \approx a \sqrt{\frac{C}{M}} \times 1 = a \sqrt{\frac{C}{M}}.$$

Hence

$$\boxed{v_{\text{ph}}(k) \rightarrow a \sqrt{\frac{C}{M}} \quad \text{and} \quad v_{\text{g}}(k) \rightarrow a \sqrt{\frac{C}{M}} \quad \text{as } k \rightarrow 0,}$$

showing that the phase and group velocities coincide for very long wavelengths.