

1. In classical mechanics, it is straightforward to define the concept of a particle flux. If there are N particles per unit length and each one has speed u in the positive x direction, then all particles in a length $u\Delta t$ will pass a fixed point in time interval Δt . The number passing a fixed point per unit time is the particle flux $\mathcal{F} = Nu\Delta t/\Delta t = Nu$. In quantum mechanics, the definition of particle flux is equally simple, provided we are dealing with wavefunctions of particles with definite momentum (i.e. momentum eigenfunctions). Consider a stream of particles represented by the wave function $\psi(x) = Ae^{ikx}$. The function $p(x) = |\psi(x)|^2$ represents the probability density when ψ is the wavefunction for a single particle. However, when ψ represents a set of particles, the function $p(x) = |\psi(x)|^2$ gives the average particle density at the position x . $p(x)$ is then the particle density function. Then, the average number of particles per unit length is the constant $|A|^2$, and their speed u is obtained from the momentum magnitude: $p = \hbar k$ and $u = p/m$, so that $u = \hbar k/m$. Since $k > 0$, so is u . The flux is found to be

$$\mathcal{F} = |A|^2 \frac{\hbar k}{m}. \quad (1)$$

A word of warning is necessary here! The flux relation (1) can only be used when the wavefunction is a momentum eigenfunction; the momentum is then the same for all the particles, and the average number of particles per unit length is a constant, independent of position. Electrons accelerated by a constant potential difference of 5 V are moving in the positive x -direction. There are on average 10^7 electrons per mm. (i) What is the wave function of the stream of electrons? (ii) What is the flux of electrons? (iii) What is the corresponding current in amperes? [Hint: The current is the total charge in coulombs passing a point per second; throughout neglect relativistic effects.]

2. A particle of mass m is confined to a one-dimensional region $0 \leq x \leq a$ (an infinite square well potential). At $t = 0$ its normalized wave function is

$$\Psi(x, t = 0) = \sqrt{\frac{8}{5a}} \left[1 + \cos\left(\frac{\pi x}{a}\right) \right] \sin\left(\frac{\pi x}{a}\right).$$

For an infinite square well we have

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}, \quad E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}, \quad n = 1, 2, 3, \dots$$

Any arbitrary wave function can be expanded in this basis, that is

$$\Psi(x, t) = \sum_n A_n e^{-iE_n t/\hbar} \psi_n(x).$$

Then $\Psi(x, t = 0)$ can be rewritten as

$$\Psi(x, t = 0) = \sqrt{\frac{8}{5a}} \left[1 + \cos\left(\frac{\pi x}{a}\right) \right] \sin\left(\frac{\pi x}{a}\right)$$

$$\begin{aligned}
&= \sqrt{\frac{8}{5a}} \sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{2}{5a}} \sin\left(\frac{\pi x}{a}\right) \\
&= \sqrt{\frac{4}{5}} \psi_1(x) + \sqrt{\frac{1}{5}} \psi_2(x)
\end{aligned}$$

which is a sum of eigenfunctions. (i) What is the wave function at a later time $t = t_0$? (ii) What is the average energy of the system at $t = 0$ and $t = t_0$? What is the probability that the particle is found in the left half of the box (i.e., in the region $0 \leq x \leq a/2$) at $t = t_0$?

3. Consider the bound state problem $E < V_0$ in the asymmetric infinite well potential

$$V(x) = \begin{cases} \infty & x \leq 0 \\ 0 & 0 < x < L \\ V_0 & L < x < 2L \\ \infty & x > 2L \end{cases} . \quad (2)$$

(i) Solve the time-dependent Schrödinger equations in regions I ($0 < x < L$) and II ($L < x < 2L$) and impose appropriate boundary conditions. (ii) Use the results in (i) to derive an equation in terms of E , V_0 , L whose solution will determine the possible energy eigenvalues E . (iii) Duplicate the procedure to determine an equation in terms of E , V_0 , L whose solution will resolve the possible energy eigenvalues for $E > V_0$.

4. Consider the square well of width a which is infinite on the left side and finite on the right,

$$V(x) = \begin{cases} \infty & x < 0 \\ 0 & 0 < x < L \\ V_0 & x > L \end{cases} . \quad (3)$$

(i) Apply appropriate boundary conditions and derive the transcendental equation that determines the energy eigenvalues for the bound states. (ii) Show that if the parameter $2mL^2V_0/\hbar^2$ is smaller than a critical value, there are no bound states. What is this critical value?

5. Consider a “downstep” potential, which drops at $x = 0$ as one goes from left to right.

$$V(x) = \begin{cases} 0 & x < 0 \\ -V_0 & x > 0 \end{cases} . \quad (4)$$

A particle of mass m and kinetic energy $E > 0$ approaches the abrupt potential drop. (i) Derive the reflection and transmission coefficients in terms of E and V_0 . (ii) When a free neutron enters a nucleus, it experiences a sudden drop in potential energy, from $V = 0$ outside to around -12 MeV inside. Suppose a neutron, emitted with kinetic energy 4 MeV by a fission event, strikes such a nucleus. What is the probability it will be absorbed, thereby initiating another fission? [*Hint:* The transmission coefficient expresses the probability of transmission through the surface.]

SOLUTIONS

1. In an electron gun, electrons are boiled off the surface of a hot metal plate. They leave the plate with very small speeds, and then the electric field accelerates them towards the anode. You can calculate the speed of the electrons by thinking of the energy changes in the system. Each electron has a charge of e coulombs, and the potential difference between the filament and the anode is V volts. The electrical energy transferred to each coulomb of charge is V joules. So the energy transferred to electrons is eV joules. The electrons gain kinetic energy. Unlike electrons in a wire, these electrons have nothing to hit, nothing to lose energy to, as they travel towards the anode. So each electron gains kinetic energy equal to the amount of energy transferred from the electrical supply. The electron starts from rest (near enough) so the kinetic energy gained is given by $mu^2/2$ where m is its mass and u is its speed. So we can say that $mu^2/2 = eV$. The mass of the electron is $m = 9 \times 10^{-31}$ kg and the electron charge is $e = 1.6 \times 10^{-19}$ C. For an electron gun with a voltage between its cathode and anode of $V = 5$ V the electrons will have a speed of about $u = 1.3 \times 10^6$ m/s. (Relativistic effects have not been taken into account.) There will be no more acceleration once the electrons have passed through the anode. (i) $\psi(x) = 3 \times 10^3 \text{ mm}^{-1/2} \exp [i 1.8 \times 10^9 \text{ m}^{-1} \cdot x]$ (ii) Since there are 10^{10} electron per meter, the flux is $\mathcal{F} \sim 1.3 \times 10^{16} \text{ s}^{-1}$. (iii) The current is $i = Nqu = 2 \times 10^{-3} \text{ A} = 1 \text{ mA}$.

2. (i) At time t_0 we have

$$\Psi(x, t_0) = \sqrt{\frac{4}{5}} e^{-iE_1 t_0/\hbar} \psi_1(x) + \sqrt{\frac{1}{5}} e^{-iE_2 t_0/\hbar} \psi_2(x).$$

(ii) The average energy does not change so that

$$\langle E \rangle = \langle \psi | \hat{H} | \psi \rangle = \sum_n E_n |A_n|^2 = E_1 |A_1|^2 + E_2 |A_2|^2 = \frac{4}{5} E_1 + \frac{1}{5} E_2 = \frac{4\pi^2 \hbar^2}{5ma^2}.$$

(iii) The probability that the particle is in the region $0 \leq x \leq a/2$ at $t = t_0$ is

$$P(0 \leq x \leq a/2; t_0) = \int_0^{a/2} |\Psi(x, t_0)|^2 dx,$$

where

$$\begin{aligned} |\Psi(x, t_0)|^2 &= \left| e^{-iE_1 t_0/\hbar} \left\{ \sqrt{\frac{8}{5a}} \sin\left(\frac{\pi x}{a}\right) \left[1 + \cos\left(\frac{\pi x}{a}\right) e^{-i(E_2 - E_1)t_0/\hbar} \right] \right\} \right|^2 \\ &= \frac{8}{5a} \sin^2\left(\frac{\pi x}{a}\right) \left[1 + \cos^2\left(\frac{\pi x}{a}\right) + 2 \cos\left(\frac{\pi x}{a}\right) \cos\left(\frac{3\pi^2 \hbar^2 t_0}{2ma^2}\right) \right], \end{aligned}$$

so that

$$P(0 \leq x \leq a/2; t_0) = \frac{1}{2} + \frac{16}{15\pi} \cos\left(\frac{3\pi^2 \hbar^2 t_0}{2ma^2}\right).$$

3. For $E < V_0$, the solutions for zones I and II are

$$\psi_I(x) = A \sin(kx) + B \cos(kx) \quad \text{and} \quad \psi_{II}(x) = C e^{-\kappa x} + D e^{\kappa x}, \quad (5)$$

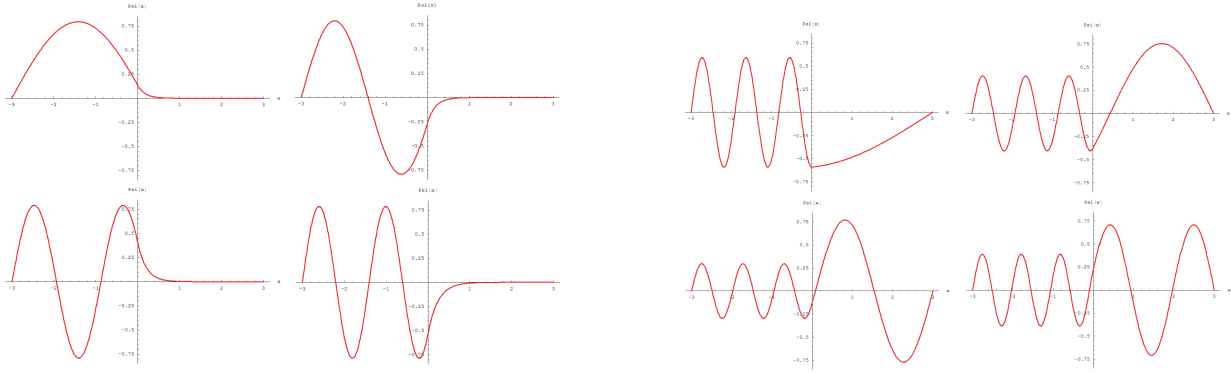


Figure 1: The first four energy eigenstates for the asymmetric infinite square well with $E < V_0$ (left) and $E > V_0$ (right). In all of the images we have taken $\hbar = 2m = 1$, $V_0 = 33$, and $L = 3$.

where $k = \sqrt{2mE}/\hbar$ and $\kappa = \sqrt{2m(V_0 - E)}/\hbar$. Imposing the boundary conditions we have

$$\psi_I(x = 0) = 0 \Rightarrow B = 0, \quad (6)$$

$$\psi_{II}(x = 2L) = 0 \Rightarrow Ce^{-2\kappa L} + De^{2\kappa L} = 0 \Rightarrow D = -Ce^{-4\kappa L}. \quad (7)$$

Imposing continuity of the wave function at $x = L$ we obtain

$$\psi_I(x = L) = \psi_{II}(x = L) \Rightarrow A \sin kL = Ce^{-\kappa L} + De^{\kappa L} \quad (8)$$

and

$$\psi'_I(x = L) = \psi'_{II}(x = L) \Rightarrow Ak \cos kL = \kappa (-Ce^{-\kappa L} + De^{\kappa L}). \quad (9)$$

Substituting the expression for D in (8) and (9) we have

$$A \sin(kL) = C(e^{-\kappa L} - e^{-3\kappa L}) \quad \text{and} \quad Ak \cos kL = -C\kappa(e^{-\kappa L} + e^{-3\kappa L}). \quad (10)$$

Taking the ratio of these two expressions we get

$$\kappa \tan(kL) = -k \frac{1 - e^{-2\kappa L}}{1 + e^{-2\kappa L}}, \quad \text{orequivalently} \quad \kappa \tan(kL) = -k \tanh(2\kappa L). \quad (11)$$

(iii) For $E > V_0$, the solutions for zones I and II are

$$\psi_I(x) = A \sin(k_1 x) \quad \text{and} \quad \psi_{II}(x) = B \sin(k_2 x). \quad (12)$$

Imposing the continuity condition on $\psi(x)$ and $\psi'(x)$ at $x = L$ we obtain

$$k_2 \tan(k_1 L) = -k_1 \tan(k_2 2L). \quad (13)$$

In Fig. 1 we show the first four eigenstates for $E < 0$ and $E > 0$.

4. The wavefunction $\psi(x)$ for a particle with energy E in a potential $V(x)$ satisfies the Schrödinger equation. Inside the well ($0 \leq x \leq L$), the particle is free. The wave function is $\psi_I(x) = A \sin(kx)$, where $k = \sqrt{2mE}/\hbar$. Outside the well ($L < x < \infty$), the potential has constant value $V > E$.

The wave function is $\psi_{II}(x) = Be^{-\kappa x}$, where $\kappa = \sqrt{2m(V_0 - E)}/\hbar$. $\psi(x)$ and its derivative are continuous at $x = L$, then $A \sin kL = Be^{-\kappa L}$ and $Ak \cos kL = -B\kappa e^{-\kappa L}$, from which

$$k \cot kL = -\kappa. \quad (14)$$

Now, since $\cot^2 \theta + 1 = \csc^2 \theta$, (14) can be rewritten as $k^2(\csc^2 \theta - 1) = -\kappa^2$, where $\theta = kL$. After some algebra the transcendental equation can be rewritten as

$$\theta \csc \theta = \pm a, \quad (15)$$

where $a = \sqrt{2mV_0L^2}/\hbar$. Note that (15) are equations for the allowed values of k . The equation with the positive sign yields values of θ in the second quadrant. The equation with the negative sign yields values of θ in the fourth quadrant. Since $\sin \theta \leq \theta \forall \theta$, it follows from (15) that there are no bound states if $2mV_0L^2/\hbar^2 \leq 1$.

5. (i) In region I, where $x < 0$, Schrödinger equation is given by

$$\frac{\partial^2 \psi_I}{\partial x^2} + \frac{2mE}{\hbar^2} \psi_I = 0 \Rightarrow \psi_I = Ae^{ik_1x} + Be^{-ik_1x}, \quad (16)$$

while in region II, where $x > 0$, we have

$$\frac{\partial^2 \psi_{II}}{\partial x^2} + \frac{2m(E + V_0)}{\hbar^2} \psi_{II} = 0 \Rightarrow \psi_{II} = Ce^{ik_2x}. \quad (17)$$

Demanding continuity of ψ and ψ' at $x = 0$ we obtain

$$\psi_I(x=0) = \psi_{II}(x=0) \Rightarrow A + B = C \quad (18)$$

and

$$\psi'_I(x=0) = \psi'_{II}(x=0) \Rightarrow ik_1(A - B) = ik_2C \quad (19)$$

Substituting (18) into (19) we get

$$ik_1(A - B) = ik_2(A + B) \quad \text{or equivalently} \quad A(k_1 - k_2) = B(k_1 + k_2). \quad (20)$$

This leads to $B/A = (k_1 - k_2)/(k_1 + k_2)$. The reflection coefficient is then

$$R = \left| \frac{B}{A} \right|^2 = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2 = \left(\frac{\sqrt{E} - \sqrt{E + V_0}}{\sqrt{E} + \sqrt{E + V_0}} \right)^2, \quad (21)$$

whereas the transmissivity is given by

$$T = 1 - R = \frac{4k_1k_2}{(k_1 + k_2)^2} = \frac{4\sqrt{E(E + V_0)}}{(\sqrt{E + V_0} + \sqrt{E})^2}. \quad (22)$$

(ii) Taking $V_0 = 12$ MeV and $E = 4$ MeV we obtain $T = 8/9$.