

Homework #7, problem 23, 29, 31, 33, 35 in chapter 6; 2, 4 in chapter 7

6-23 Inside the well, the particle is free and the Schrödinger waveform is trigonometric with wavenumber $k = \left(\frac{2mE}{\hbar^2}\right)^{1/2}$:

$$\psi(x) = A \sin kx + B \cos kx \quad 0 \leq x \leq L.$$

The infinite wall at $x = 0$ requires $\psi(0) = B = 0$. Beyond $x = L$, $U(x) = U$ and the Schrödinger equation

$$\frac{d^2\psi}{dx^2} = \left(\frac{2m}{\hbar^2}\right)\{U - E\}\psi(x), \text{ which has exponential solutions for } E < U$$

$$\psi(x) = Ce^{-\alpha x} + De^{+\alpha x}, \quad x > L$$

where $\alpha = \left[\frac{2m(U-E)}{\hbar^2}\right]^{1/2}$. To keep ψ bounded at $x = \infty$ we must take $D = 0$. At $x = L$,

continuity of ψ and $\frac{d\psi}{dx}$ demands

$$A \sin kL = Ce^{-\alpha L}$$

$$kA \cos kL = -\alpha Ce^{-\alpha L}$$

Dividing one by the other gives an equation for the allowed particle energies: $k \cot kL = -\alpha$. The dependence on E (or k) is made more explicit by noting that $k^2 + \alpha^2 = \frac{2mU}{\hbar^2}$, which allows the

energy condition to be written $k \cot kL = -\left[\left(\frac{2mU}{\hbar^2}\right) - k^2\right]^{1/2}$. Multiplying by L , squaring the result,

and using $\cot^2 \theta + 1 = \csc^2 \theta$ gives $(kL)^2 \csc^2(kL) = \frac{2mUL^2}{\hbar^2}$ from which we obtain

$\frac{kL}{\sin kL} = \left(\frac{2mUL^2}{\hbar^2}\right)^{1/2}$. Since $\frac{\theta}{\sin \theta}$ is never smaller than unity for any value of θ , there can be no

bound state energies if $\frac{2mUL^2}{\hbar^2} < 1$.

6-29 (a) Normalization requires $1 = \int_{-\infty}^{\infty} |\psi|^2 dx = C^2 \int_0^{\infty} e^{-2x} (1 - e^{-x})^2 dx = C^2 \int_0^{\infty} (e^{-2x} - 2e^{-3x} + e^{-4x}) dx$.

The integrals are elementary and give $1 = C^2 \left\{ \frac{1}{2} - 2\left(\frac{1}{3}\right) + \frac{1}{4} \right\} = \frac{C^2}{12}$. The proper units for C are those of $(\text{length})^{-1/2}$ thus, normalization requires $C = (12)^{1/2} \text{ nm}^{-1/2}$.

(b) The most likely place for the electron is where the probability $|\psi|^2$ is largest. This is also where ψ itself is largest, and is found by setting the derivative $\frac{d\psi}{dx}$ equal zero:

$$0 = \frac{d\psi}{dx} = C \{-e^{-x} + 2e^{-2x}\} = Ce^{-x} \{2e^{-x} - 1\}.$$

The RHS vanishes when $x = \infty$ (a minimum), and when $2e^{-x} = 1$, or $x = \ln 2 \text{ nm}$. Thus, the most likely position is at $x_p = \ln 2 \text{ nm} = 0.693 \text{ nm}$.

(c) The average position is calculated from

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi|^2 dx = C^2 \int_0^{\infty} x e^{-2x} (1 - e^{-x})^2 dx = C^2 \int_0^{\infty} x (e^{-2x} - 2e^{-3x} + e^{-4x}) dx.$$

The integrals are readily evaluated with the help of the formula $\int_0^{\infty} x e^{-ax} dx = \frac{1}{a^2}$ to get

$$\langle x \rangle = C^2 \left\{ \frac{1}{4} - 2 \left(\frac{1}{9} \right) + \frac{1}{16} \right\} = C^2 \left\{ \frac{13}{144} \right\}. \text{ Substituting } C^2 = 12 \text{ nm}^{-1} \text{ gives}$$

$$\langle x \rangle = \frac{13}{12} \text{ nm} = 1.083 \text{ nm}.$$

We see that $\langle x \rangle$ is somewhat greater than the most probable position, since the probability density is skewed in such a way that values of x larger than x_p are weighted more heavily in the calculation of the average.

6-31 The symmetry of $|\psi(x)|^2$ about $x = 0$ can be exploited effectively in the calculation of average values. To find $\langle x \rangle$

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx$$

We notice that the integrand is antisymmetric about $x = 0$ due to the extra factor of x (an odd function). Thus, the contribution from the two half-axes $x > 0$ and $x < 0$ cancel exactly, leaving $\langle x \rangle = 0$. For the calculation of $\langle x^2 \rangle$, however, the integrand is symmetric and the half-axes contribute equally to the value of the integral, giving

$$\langle x \rangle = \int_0^{\infty} x^2 |\psi|^2 dx = 2C^2 \int_0^{\infty} x^2 e^{-2x/x_0} dx.$$

Two integrations by parts show the value of the integral to be $2 \left(\frac{x_0}{2} \right)^3$. Upon substituting for C^2 ,

we get $\langle x^2 \rangle = 2 \left(\frac{1}{x_0} \right) (2) \left(\frac{x_0}{2} \right)^3 = \frac{x_0^2}{2}$ and $\Delta x = (\langle x^2 \rangle - \langle x \rangle^2)^{1/2} = \left(\frac{x_0^2}{2} \right)^{1/2} = \frac{x_0}{\sqrt{2}}$. In calculating the probability for the interval $-\Delta x$ to $+\Delta x$ we appeal to symmetry once again to write

$$P = \int_{-\Delta x}^{+\Delta x} |\psi|^2 dx = 2C^2 \int_0^{\Delta x} e^{-2x/x_0} dx = -2C^2 \left(\frac{x_0}{2} \right) e^{-2x/x_0} \Big|_0^{\Delta x} = 1 - e^{-\sqrt{2}} = 0.757$$

or about 75.7% independent of x_0 .

- 6-33 (a) Since there is no preference for motion in the leftward sense vs. the rightward sense, a particle would spend equal time moving left as moving right, suggesting $\langle p_x \rangle = 0$.
- (b) To find $\langle p_x^2 \rangle$ we express the average energy as the sum of its kinetic and potential energy contributions: $\langle E \rangle = \langle \frac{p_x^2}{2m} \rangle + \langle U \rangle = \frac{\langle p_x^2 \rangle}{2m} + \langle U \rangle$. But energy is sharp in the oscillator ground state, so that $\langle E \rangle = E_0 = \frac{1}{2} \hbar \omega$. Furthermore, remembering that $U(x) = \frac{1}{2} m \omega^2 x^2$ for the quantum oscillator, and using $\langle x^2 \rangle = \frac{\hbar}{2m\omega}$ from Problem 6-32, gives $\langle U \rangle = \frac{1}{2} m \omega^2 \langle x^2 \rangle = \frac{1}{4} \hbar \omega$. Then $\langle p_x^2 \rangle = 2m(E_0 - \langle U \rangle) = 2m\left(\frac{\hbar \omega}{4}\right) = \frac{m\hbar \omega}{2}$.

(c)
$$\Delta p_x = (\langle p_x^2 \rangle - \langle p_x \rangle^2)^{1/2} = \left(\frac{m\hbar \omega}{2}\right)^{1/2}$$

6-35 Applying the momentum operator $[p_x] = \left(\frac{\hbar}{i}\right) \frac{d}{dx}$ to each of the candidate functions yields

(a)
$$[p_x]\{A \sin(kx)\} = \left(\frac{\hbar}{i}\right)k\{A \cos(kx)\}$$

(b)
$$[p_x]\{A \sin(kx) - A \cos(kx)\} = \left(\frac{\hbar}{i}\right)k\{A \cos(kx) + A \sin(kx)\}$$

(c)
$$[p_x]\{A \cos(kx) + iA \sin(kx)\} = \left(\frac{\hbar}{i}\right)k\{-A \sin(kx) + iA \cos(kx)\}$$

(d)
$$[p_x]\{e^{ik(x-a)}\} = \left(\frac{\hbar}{i}\right)ik\{e^{ik(x-a)}\}$$

In case (c), the result is a multiple of the original function, since

$$-A \sin(kx) + iA \cos(kx) = i\{A \cos(kx) + iA \sin(kx)\}.$$

The multiple is $\left(\frac{\hbar}{i}\right)(ik) = \hbar k$ and is the eigenvalue. Likewise for (d), the operation $[p_x]$ returns the original function with the multiplier $\hbar k$. Thus, (c) and (d) are eigenfunctions of $[p_x]$ with eigenvalue $\hbar k$, whereas (a) and (b) are not eigenfunctions of this operator.

- 7-2 (a) To the left of the step the particle is free with kinetic energy E and corresponding wavenumber $k_1 = \left(\frac{2mE}{\hbar^2}\right)^{1/2}$:

$$\psi(x) = Ae^{ik_1x} + Be^{-ik_1x} \quad x \leq 0$$

To the right of the step the kinetic energy is reduced to $E - U$ and the wavenumber is

$$\text{now } k_2 = \left[\frac{2m(E-U)}{\hbar^2} \right]^{1/2}$$

$$\psi(x) = Ce^{ik_2x} + De^{-ik_2x} \quad x \geq 0$$

with $D = 0$ for waves incident on the step from the left. At $x = 0$ both ψ and $\frac{d\psi}{dx}$ must

be continuous: $\psi(0) = A + B = C$

$$\left. \frac{d\psi}{dx} \right|_0 = ik_1(A - B) = ik_2C.$$

(b) Eliminating C gives $A + B = \frac{k_1}{k_2}(A - B)$ or $A\left(\frac{k_1}{k_2} - 1\right) = B\left(\frac{k_1}{k_2} + 1\right)$. Thus,

$$R = \left| \frac{B}{A} \right|^2 = \frac{(k_1/k_2 - 1)^2}{(k_1/k_2 + 1)^2} = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}$$

$$T = 1 - R = \frac{4k_1k_2}{(k_1 + k_2)^2}$$

(c) As $E \rightarrow U$, $k_2 \rightarrow 0$, and $R \rightarrow 1$, $T \rightarrow 0$ (no transmission), in agreement with the result for any energy $E < U$. For $E \rightarrow \infty$, $k_1 \rightarrow k_2$ and $R \rightarrow 0$, $T \rightarrow 1$ (perfect transmission) suggesting correctly that very energetic particles do not *see* the step and so are unaffected by it.

7-4 The reflection coefficient for this case is given in Problem 7-2 as

$$R = \left| \frac{B}{A} \right|^2 = \frac{(k_1/k_2 - 1)^2}{(k_1/k_2 + 1)^2} = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}.$$

The wavenumbers are those for electrons with kinetic energies $E = 54.0$ eV and $E - U = 54.0$ eV + 10.0 eV = 64.0 eV:

$$\frac{k_1}{k_2} = \left(\frac{E}{E-U} \right)^{1/2} = \left(\frac{54 \text{ eV}}{64 \text{ eV}} \right)^{1/2} = 0.9186.$$

Then, $R = \frac{(0.9186 - 1)^2}{(0.9186 + 1)^2} = 1.80 \times 10^{-3}$ is the fraction of the incident beam that is reflected at the boundary.

Reflected current: $0.1 \times 1.8 \times 10^{-3} = 1.8 \times 10^{-4}$ mA