Solution to HW#3

1. Reed: Chapter 3

Problem 3-3

Using classical arguments, derive an expression for the speed \( v \) of a particle in a one-dimensional infinite potential well. Apply your result to the case of an electron in a well with \( L = 1\,\text{Å} \). For what value of \( n \) does \( v \) exceed the speed of light? To what energy does this correspond?

By equating the energy of a particle in state \( n \) of an infinite well to the classical kinetic energy \( \frac{mv^2}{2} \),

\[
E = \frac{n^2 \hbar^2}{8mL^2} = \frac{mv^2}{2},
\]

we find

\[
v = \frac{n\hbar}{2mL}.
\]

For an electron in a well with \( L = 1\,\text{Å} \), this gives \( v = (3.637 \times 10^6 \, n) \, \text{m/sec} \); \( v \) exceeds \( c \) for \( n \sim 82 \), which corresponds to an energy of 259 kV.
2. Reed: Chapter 3

**Problem 3-5**

A particle in some potential is described by the wavefunction \( \psi(x) = Axe^{kx} \) \((0 \leq x < \infty; \ k > 0; \) see Problem 2-5.) If \( k = 0.5 \text{Å}^{-1} \), what is the probability of finding the particle between \( x = 2.0 \) and \( 2.1 \text{Å} \)?

From Problem 2.5 the normalization of this wavefunction is given by \( A^2 = 4k^3 \). Hence

\[
\Psi(x) = Axe^{-kx} \text{ from } x > 0
\]

\[
P = \int_{x_1}^{x_2} \Psi^* \Psi\,dx = \int_{x_1}^{x_2} A^2 x^2 e^{-2kx} \,dx
\]

Using integrals from Appendix C:

\[
P = \frac{A^2}{4k^3} \left( -e^{-2kx_2} \left( 2k^2 x^2 + 2kx + 1 \right) \right) \bigg|_{x_1}^{x_2}
\]

Plugging in expression for \( A \) above and values: \( k=0.5 \text{ Å} \), \( x_1 = 2.0 \text{ Å} \) and \( x_2 = 2.1 \text{ Å} \) one gets:

\[
P = 0.0271 \text{ or } 2.71\%
\]

\[
P(x, x + \Delta x) = \psi^2(x)\,\Delta x = \left( A^2 x^2 e^{-2kx} \right)\,\Delta x = \left( 4k^3 x^2 e^{-2kx} \right)\,\Delta x
\]

\[
= \left\{ 4(0.5\text{Å}^{-1})^3 (2\text{Å})^2 \exp\left[-2(0.5\text{Å}^{-1})(2.0\text{Å})\right] \right\} (0.1\text{Å}) = 0.0271.
\]
Problem 3-9

A proton is moving within a nuclear potential of depth 25 MeV and full width \(2L = 10^{-14}\) meters. If the potential can be modeled as a finite rectangular well, how many energy states are available to the proton?

The number of states is given by

\[ N(K) = 1 + \left[ \frac{2K}{\pi} \right] = 1 + \left[ \frac{2}{\pi} \sqrt{\frac{2mV_0L^2}{\hbar^2}} \right], \]

where the square brackets designate the largest integer less than or equal to the argument within. With \(V_0 = 25\) MeV = \(4.00 \times 10^{-12}\) J, \(L = 0.5 \times 10^{-14}\) m, and a proton \((1.67 \times 10^{-27}\) kg),

\[ N(K) = 1 + \left[ \frac{2}{\pi} \sqrt{\frac{2(1.67 \times 10^{-27})(4.00 \times 10^{-12})(0.5 \times 10^{-14})^2}{(1.055 \times 10^{-34})^2}} \right] \]

\[ = 1 + [3.487] = 4. \]

Only four energy states are available to the proton in this situation.
Problem 3-11

Consider a particle of mass $m$ moving in the "semi-infinite" potential well illustrated below. Set up and solve the SWE for this system; assume $E < V_o$. Applying the appropriate boundary conditions at $x = 0$ and $x = L$, derive an expression for the permissible energy eigenvalues. With $V_o = 10$ eV, $L = 5\text{Å}$ and $m = m_{\text{electron}}$, compute the values of the energy (in eV) for the two lowest bound states.
Define region 1 as that for which $x < 0$, region 2 as $0 \leq x \leq L$, and region 3 as $x > L$. Since $V = \infty$ in region 1, $\psi = 0$ there. We restrict attention to bound states, that is, $E < V_o$. In regions 2 and 3 the solutions of the Schrödinger equation take the usual sinusoidal and exponential forms:

$$\psi_2 = A \cos(k_2 x) + B \sin(k_2 x), \quad k_2 = \sqrt{2mE/\hbar^2}$$

and

$$\psi_3 = C \exp(k_3 x) + D \exp(-k_3 x), \quad k_3 = \sqrt{2m(V_o - E)/\hbar^2}.$$

At $x = 0$, we must have $\psi_2 = 0$, which forces $A = 0$. As $x \to \infty$, we must have $\psi_3 \to 0$, which forces $C = 0$. Demanding the continuity of $\psi_2$ and $\psi_3$ and their first derivatives at $x = L$ leads to

$$B \sin(k_2 L) = D \exp(-k_3 L)$$

and

$$k_2 B \cos(k_2 L) = -k_3 D \exp(-k_3 L).$$

Dividing the first of these conditions by the second (or vice-versa) gives the energy eigenvalue condition

$$-k_3 \tan(k_2 L) = k_2.$$

Defining dimensionless variables $\xi = k_2 L$ and $\eta = k_3 L$, this condition can be expressed as

$$-\eta \tan(\xi) = \xi,$$

$\xi$ and $\eta$ also satisfy

$$\xi^2 + \eta^2 = \frac{2mV_o L^2}{\hbar^2} = K^2.$$

For the values specified, $K^2 = 65.561$. This result can be used to eliminate $\eta$ (or $\xi$) from the eigenvalue equation, leaving

$$-\sqrt{65.561 - \xi^2} \tan(\xi) = \xi.$$

The first two roots of this equation are $\xi_1 = 2.78983$ and $\xi_2 = 5.53117$; these correspond to energies of 1.187 and 4.667 eV, respectively.
Derive an expression analogous to equation (3.4.11) for the odd-parity states of the finite rectangular well.

For the odd-parity states of the finite rectangular well we have ($F = -C$)

\[
\begin{align*}
\psi_1(x) &= C e^{k_1x} \\
\psi_2(x) &= A \sin(k_2x) \\
\psi_3(x) &= -C e^{-k_1x}
\end{align*}
\]

($x < -L$)

($-L \leq x \leq L$)

($x > L$).

The boundary conditions demand

\[-A \sin \xi = Ce^{-\eta}\]

and

\[k_2 A \cos \xi = k_1 C e^{-\eta}.\]

(We do not actually use this latter condition). From the first of these we can write

\[C^2 = A^2 \sin^2 \xi \ e^{2\eta}.\]

Normalizing the wavefunction demands

\[\int_{-\infty}^{-L} \psi_1^* \psi_1 \, dx + \int_{-L}^{L} \psi_2^* \psi_2 \, dx + \int_{L}^{\infty} \psi_3^* \psi_3 \, dx = 1,
\]

or

\[C^2 \int_{-\infty}^{-L} e^{2k_1x} \, dx + A^2 \int_{-L}^{L} \sin^2(k_2x) \, dx + C^2 \int_{L}^{\infty} e^{-2k_1x} \, dx = 1.
\]

The first and third integrals are identical. The normalization condition reduces to

\[\frac{C^2 e^{-2\eta}}{k_1} + A^2 \left[ L - \frac{\sin(2\xi)}{2k_2} \right] = 1.
\]

Eliminating $A^2$ via the boundary-condition information and solving for $C^2$ gives

\[C^2 = \frac{\eta \xi \ e^{2\eta}}{L \left[ \xi + \eta \xi \csc^2 \xi - \eta \cot \xi \right]}.
\]

The probability of finding the particle outside the confines of the well is then given by
\[ P_{out}^{\text{add}} = \int_{-L}^{L} \psi_1^* \psi_1 \, dx + \int_{L}^{\infty} \psi_3^* \psi_3 \, dx = \frac{C^2 \, e^{-2\eta}}{k_1} = \frac{\eta \xi \, e^{2\eta}}{L \left[ \xi + \eta \xi \csc^2 \xi - \eta \cot \xi \right]} \frac{e^{-2\eta}}{k_1}, \]

or, since \( k_1 L = \eta \),

\[ P_{out}^{\text{add}} = \frac{\xi}{\left[ \xi + \eta \xi \csc^2 \xi - \eta \cot \xi \right]} . \]
Problem 3-14

For the system discussed in example 3.2, determine the probability of finding the particle outside the well for each of the four possible bound states.

Even parity states are $\xi_1 = 1.3118$ and $\xi_3 = 3.8593$
Odd parity states are $\xi_2 = 2.6076$ and $\xi_4 = 4.9603$

From equation 3.4.11 (for even-parity), the solution to problem 3-12 (for odd-parity) and the values in Example 3.2, we find that:

<table>
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<tr>
<th>State</th>
<th>Parity</th>
<th>$\xi$</th>
<th>$\eta$</th>
<th>Probability</th>
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<tbody>
<tr>
<td>1</td>
<td>Even</td>
<td>1.3118</td>
<td>4.9523</td>
<td>0.0110</td>
</tr>
<tr>
<td>2</td>
<td>Odd</td>
<td>2.6076</td>
<td>4.4098</td>
<td>0.0479</td>
</tr>
<tr>
<td>3</td>
<td>Even</td>
<td>3.8597</td>
<td>3.3688</td>
<td>0.1298</td>
</tr>
<tr>
<td>4</td>
<td>Odd</td>
<td>4.9630</td>
<td>1.2708</td>
<td>0.4133</td>
</tr>
</tbody>
</table>

Note that the higher the energy, the more likely you are to find the particle outside the box.