E&R - Ch. 5, Problem 23

For the particle moving in a potential V(x), which is shown in Figure 5-22, a particle will either be confined and have discrete energy levels, not confined and have a continuum of allowed energy values, or be below the potential which indicates that no allowed energy values exist.

Part A $E < V_0$, there are no allowed values of *E* (negative KE if there were allowed states).

Part B $V_0 < E < V_1$, the particle is confined and there are discrete values for the allowed *E*.

Part C $V_1 < E < V_2$, the particle is confined and there are discrete values for the allowed *E*.

Part D $V_2 < E < V_3$, the particle is not confined and there are a continuum of allowed values for *E*.

Part E $V_3 <$, the particle is not confined and there are a continuum of allowed values for *E*.

E&R - Ch. 6, Problem 12

The exponential general solutions are:

$$\psi_I(x) = C \exp(k_{II}x) + D \exp(-k_{II}x)$$

$$\psi_{III}(x) = F \exp(k_{II}x) + G \exp(-k_{II}x)$$

where

$$k_{II} = \sqrt{\frac{2m(V_o - E)}{\hbar^2}}$$

Let's start with $\psi_I(x)$. Substituting this into the time-independent Schrödinger equation results in:

$$\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} = [V_o - E] \psi(x)$$
$$\frac{\hbar^2}{2m} k_{II}^2 \left(C \exp(k_{II}x) + D \exp(-k_{II}x) \right) = [V_o - E] \left(C \exp(k_{II}x) + D \exp(-k_{II}x) \right)$$
$$\frac{\hbar^2 k_{II}^2}{2m} = [V_o - E]$$

Finally, we can substitute k_{II} into the equation above:

$$\frac{\hbar^2 k_{II}^2}{2m} = [V_o - E]$$
$$\frac{\hbar^2}{2m} \left(\frac{2m[V_o - E]}{\hbar^2}\right) = [V_o - E]$$
$$\hookrightarrow V_o - E = V_o - E$$

Therefore, $\psi_I(x)$ is a valid solution since it satisfies the time-independent Schrödinger equation.

For $\psi_{III}(x)$, substitution into the time-independent Schrödinger equation produces:

$$\frac{\hbar^2}{2m}k_{II}^2 \left(F \exp(k_{II}x) + G \exp(-k_{II}x)\right) = [V_o - E] \left(F \exp(k_{II}x) + G \exp(-k_{II}x)\right)$$
$$\frac{\hbar^2 k_{II}^2}{2m} = [V_o - E]$$

which is the same result that was found for $\psi_I(x)$. Therefore, both $\psi_I(x)$ and $\psi_{II}(x)$ are valid solutions to the time-independent Schrödinger equation.

E&R - Ch. 6, Problem 18

Due to the complex nature of having two interfaces for reflection and transmission, a set of equations needs to be used to solve for transmission from region I (x < 0) to region III (x > a). The particle has an energy of $9V_o$ and the potential function has the following form:

$$V(x) = \begin{cases} 8V_o & \text{for} & x < 0\\ 0 & \text{for} & 0 < x < a\\ 5V_o & \text{for} & x > a \end{cases}$$

With this information, we can set up the values of *k* for each region. These are:

$$\begin{aligned} k_{I} &= \sqrt{\frac{2m(9V_{o} - 8V_{o})}{\hbar^{2}}} = \sqrt{\frac{2mV_{o}}{\hbar^{2}}} \\ k_{II} &= \sqrt{\frac{2m(9V_{o} - 0)}{\hbar^{2}}} = \sqrt{\frac{2m(9V_{o})}{\hbar^{2}}} \\ k_{III} &= \sqrt{\frac{2m(9V_{o} - 5V_{o})}{\hbar^{2}}} = \sqrt{\frac{2m(4V_{o})}{\hbar^{2}}} \end{aligned}$$

These values of k can be rewritten in terms of k_I , which significantly simplifies the algebra that is used to determine various coefficients. The new values for k are then:

$$k_I = k$$
$$k_{II} = 3k$$
$$k_{III} = 2k$$

We can also define the wave functions for each region with the new *k* values:

$$\psi_{I}(x) = A \exp(ikx) + B \exp(-ikx)$$

$$\psi_{II}(x) = F \exp(-i3kx) + G \exp(i3kx)$$

$$\psi_{III}(x) = C \exp(i2kx)$$

Utilizing boundary conditions for the continuity of $\psi(x)$ across the step at x = 0 and x = a, we obtain:

$$A + B = F + G \tag{1}$$

$$F \exp(-i3ka) + G \exp(i3ka) = C \exp(i2ka)$$
(2)

The boundary conditions for continuity of $d\psi(x)/dx$ at x = 0 and x = a result in:

$$k (A + B) = 3k (F + G)$$

$$3k (G \exp (i3ka) - F \exp (-i3ka)) = 2Ck \exp (i2ka)$$

which can be simplified to:

$$A + B = 3(F + G)$$
(3)

$$3(G\exp(i3ka) - F\exp(-i3ka)) = 2C\exp(i2ka)$$
(4)

If we set $z = \exp(ika)$, the boundary condition equations (2 and 4) at the x = a interface can be written as:

$$Fz^{-3} + Gz^3 = Cz^2 (5)$$

$$3\left(Gz^3 - Fz^{-3}\right) = 2Cz^2 \tag{6}$$

The transmission coefficient can be found once we determine what (C/A) is. This can be done by working with equations 1, 3, 5 and 6, which results in:

$$\left(\frac{C}{A}\right) = \frac{6z}{10 - z^6}$$

The transmission coefficient is then:

$$T = \left(\frac{v_{III}}{v_I}\right) \frac{C^*C}{A^*A}$$
$$= \left(\frac{\hbar k_{III}}{\hbar k_I}\right) \left[\left(\frac{6z}{10 - z^6}\right)^* \left(\frac{6z}{10 - z^6}\right) \right]$$
$$= 2 \left(\frac{36z^*z}{(10 - (z^*)^6)(10 - z^6)}\right)$$

The quantity $z^*z = 1$ since *z* is a purely complex exponential. The denominator can be expressed as:

$$(10 - (z^*)^6) (10 - z^6) \hookrightarrow 100 - 10 (\exp(-i6ka) + \exp(i6ka)) + 1 \Rightarrow 101 - 10 (2\cos(6ka))$$

The transmission coefficient is then:

$$T = \frac{72}{101 - 20\cos(6ka)}$$

E&R - Ch. 6, Problem 23

For this problem, we know that the energy of a given eigenvalue is:

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

Part A To find the adjacent eigenvalue, we need to find the difference between E_n and E_{n+1} . The value of E_{n+1} is:

$$E_{n+1} = \frac{\hbar^2 \pi^2 (n+1)^2}{2ma^2}$$

The fractional difference then becomes:

$$\frac{\Delta E_n}{E_n} = \frac{E_{n+1} - E_n}{E_n}$$

$$= \frac{\frac{\hbar^2 \pi^2}{2ma^2} \left[(n+1)^2 - n^2 \right]}{\frac{\hbar^2 \pi^2 n^2}{2ma^2}}$$

$$= \frac{(n+1)^2 - n^2}{n^2}$$

$$= \frac{n^2 + 2n + 1 - n^2}{n^2}$$

$$\Rightarrow \frac{2n+1}{n^2}$$

Part B In the classical limit, energy levels are expressed as a continuum of states. This can also be expressed as the number of states $n \to \infty$. The classical limit for the fractional difference in energy between adjacent eigenvalues is then:

$$\lim_{n\to\infty}\frac{2n+1}{n^2}=0$$

which states that with a continuum of energy levels, the difference between quantized energy levels vanishes. This corresponds to a classical system where quantization is not observable.

E&R - Ch. 6, Problem 27

For the n = 1 and n = 3 states in an infinite square well potential, we have the following eigenfunctions (or wavefunctions):

$$\psi_1(x) = \cos\left(\frac{\pi x}{a}\right)$$

 $\psi_3(x) = \cos\left(\frac{3\pi x}{a}\right)$

Substituting these equations into the expression given in the problem results in:

$$\int_{-\infty}^{\infty} \psi_1(x)\psi_3(x)dx$$
$$\int_{-\infty}^{\infty} \cos\left(\frac{\pi x}{a}\right)\cos\left(\frac{3\pi x}{a}\right)dx$$
$$\frac{2}{a}\int_{-a/2}^{a/2} \cos\left(\frac{\pi x}{a}\right)\cos\left(\frac{3\pi x}{a}\right)dx$$
$$\frac{1}{a}\int_{-a/2}^{a/2} \left[\cos\left(\frac{4\pi x}{a}\right) - \cos\left(\frac{2\pi x}{a}\right)\right]dx$$

If we set $2\pi x/a = u$, then $du = 2\pi/a$ and the integral becomes:

$$\frac{1}{2\pi} \int_{-pi}^{pi} \left[\cos(2u) - \cos(u) \right] du$$
$$\frac{1}{2\pi} \left[\int_{-pi}^{pi} \cos(2u) \, du - \int_{-pi}^{pi} \cos(u) \, du \right]$$

Evaluating the integrals show that they both equal 0. Therefore,

$$\int_{-\infty}^{\infty}\psi_1(x)\psi_3(x)dx=0$$

E&R - Ch. 7, Problem 10

While the Schrödinger atom and the Bohr atom describe the electron radius in terms of a quantum number, n, Bohr suggested that electrons have a circular orbital with a definite radius. The Schrödinger atom is slightly larger since it accounts for the radial probability density for an electron with a given n (as well as m_l and l). This distribution of radii in the Schrödinger atom allows for electrons to exist with radii around the radius defined by Bohr.

E&R - Ch. 7, Problem 14

For the location of an orbiting electron, Bohr stated that the radius will be a function of *n* and the atomic number, *Z*:

$$r_{Bohr} = \frac{n^2 a_o}{Z}$$

The location of an electron in the Schrödinger atom is a probability distribution with a peak value located at r_{Bohr} , but the expected value for the radius depends on the quantum number *l*:

$$\overline{r_{n,l}} = \frac{n^2 a_o}{Z} \left(1 + \frac{1}{2} \left[1 - \frac{l(l+1)}{n^2} \right] \right)$$

Taking the case of n = 1, l = 0, we can see that the Schrödinger atom has an expected radius that is 1.5 times the size of the Bohr radius.

In terms of orbital angular momentum, Bohr postulated about a 2-D atom. In this atom, electrons required some angular momentum to maintain their radial path and gave rise to the following equation:

$$L_{Bohr} = n\hbar$$

This indicates that there will always exist some orbital angular momentum for all quantum number n. From the Schrödinger atom, orbital angular momentum is a vector that has an x, y and z component. The z component depends on m_l and lies in the direction of the principal atomic axis. These components are:

$$L_z = m_l \hbar$$
$$L = \sqrt{l(l+1)}\hbar$$

From this, we can also see that for n = 1, l and m_l are 0 and there is no orbital angular momentum for an electron.

Finally, the total energy in the Bohr and Schrödinger atoms are equal with the exception that the Schrödinger atom utilizes reduced mass (μ) instead of electron mass to account for the massive nucleus.

E&R - Ch. 7, Problem 6

From Example 7-4, we determined that the radius for the ground state (n = 1) of the hydrogen atom is the Bohr radius. This is defined as:

$$R = \frac{4\pi\epsilon_o\hbar^2}{\mu q^2} = a_o$$

Part A Having defined the stable size of the radius, we can substitute this into the expression for energy and obtain an energy for the hydrogen atom with n = 1:

$$E = \frac{\hbar^2}{2\mu R^2} - \frac{q^2}{4\pi\epsilon_o R}$$

= $\frac{\hbar^2}{2\mu} \left(\frac{\mu q^2}{4\pi\epsilon_o \hbar^2}\right)^2 - \frac{q^2}{4\pi\epsilon_o} \left(\frac{\mu q^2}{4\pi\epsilon_o \hbar^2}\right)$
= $\frac{\mu q^4}{(4\pi\epsilon_o)^2 2\hbar^2} - \frac{\mu q^4}{(4\pi\epsilon_o)^2 \hbar^2}$
= $-\frac{\mu q^4}{(4\pi\epsilon_o)^2 2\hbar^2}$

Part B We see that the equation found above is identical to Equation 7-22 when Z = 1 and n = 1. These values correspond to the ground state of a hydrogen atom.