

Problem 1

Exploring Schrödinger's equation. For each of the following potentials, use the applet <http://www.benfold.com/sse/shoot.html> to sketch the potential, determine the first four energy levels E_n , draw lines on the plot representing each energy level. Sketch the wave function using the E_n line as the x -axis for each energy level. Which energy spectrum best matches the hydrogen atom? Note this applet uses units where $\hbar^2/2m = 1$.

Part a

$$V = -19.4/(|x| + 1)$$

The first four energy levels for this potential are $E_1 = -13.66$, $E_2 = -8.36$, $E_3 = -6.25$, and $E_4 = -4.75$. These energy levels, along with their wave forms, are shown in figure 1. Of the three parts of this problem, this appears to be the best match for the hydrogen atom (see figure 2, mostly from library.thinkquest.org).

Part b

$(x/2)^2$ (quadratic), the harmonic oscillator.

The first four energy levels for this potential are $E_1 = 0.5$, $E_2 = 1.5$, $E_3 = 2.5$, and $E_4 = 3.5$. These energy levels, along with their wave forms, are shown in figure 3.

Part c

Three square wells of width 1.0, depth 15.0, and period 2.0.

The first four energy levels for this potential are $E_1 = -10.975$, $E_2 = -10.860$, $E_3 = -10.738$, $E_4 = -1.744$, and $E_5 = -1.040$. These energy levels, along with their wave forms, are shown in figure 4.

Problem 2

Approximate the hydrogen atom as an electron in an infinite square well.

Part a

Solve Schrödinger's equation with an infinite square well of width a for the energy levels E_n and normalized wave functions.

At its most basic, Schrödinger's equation is $\hat{H}\Psi = E\Psi$. However, if the potential does not depend on time (which it does not in this case), then it can be shown (and is shown in [Tipler & Lewellyn, pp. 226-227]) that this equation is a product of two equations, $\Psi(x, t) = \psi(x)\phi(t)$, that $\hat{E} = E$ is constant, and that the equation can be represented in a time independent form, $\hat{H}\psi(x) = E\psi(x)$. \hat{H} is the Hamiltonian, and can be expanded as $\hat{T} + \hat{V}$, giving us $\hat{T}\psi(x) + \hat{V}\psi(x) = E\psi(x)$. \hat{V} is just $V(x)$. \hat{T} can be expanded by recognizing that $T = \frac{p^2}{2m}$, where m in this case is constant, so $\hat{T} = \frac{\hat{p}^2}{2m}$. \hat{p} can also be expanded, recognizing that $p = \hbar k$, where \hbar is a known constant, giving us $\hat{p} = \hbar\hat{k}$, and $\hat{T} = \frac{\hbar^2\hat{k}^2}{2m}$. \hat{k} gives the x component of momentum divided by \hbar , which is $\hat{k} = \frac{1}{i} \frac{\partial}{\partial x} = -i \frac{\partial}{\partial x}$. This gives us:

$$\frac{\hbar^2}{2m} \left(-i \frac{\partial}{\partial x} \right)^2 \psi(x) + V(x)\psi(x) = E\psi(x)$$

Since we are dealing with an infinite well, we know that the probability of the particle being outside the well is zero. We also know that $V(x)$ is constant inside the infinite square well, and so we can pick $V(x) = 0$ inside the well. The time independent Schrödinger's equation inside the well becomes:

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} &= E\psi(x) \\ \frac{d^2\psi(x)}{dx^2} &= -\frac{2mE}{\hbar^2}\psi(x) \end{aligned}$$

with boundary conditions $\psi(x) = 0$ at $x = 0$ and at $x = a$. This differential equation can be solved several ways, for instance using $\psi(x) = A \sin(kx) + B \cos(kx)$.

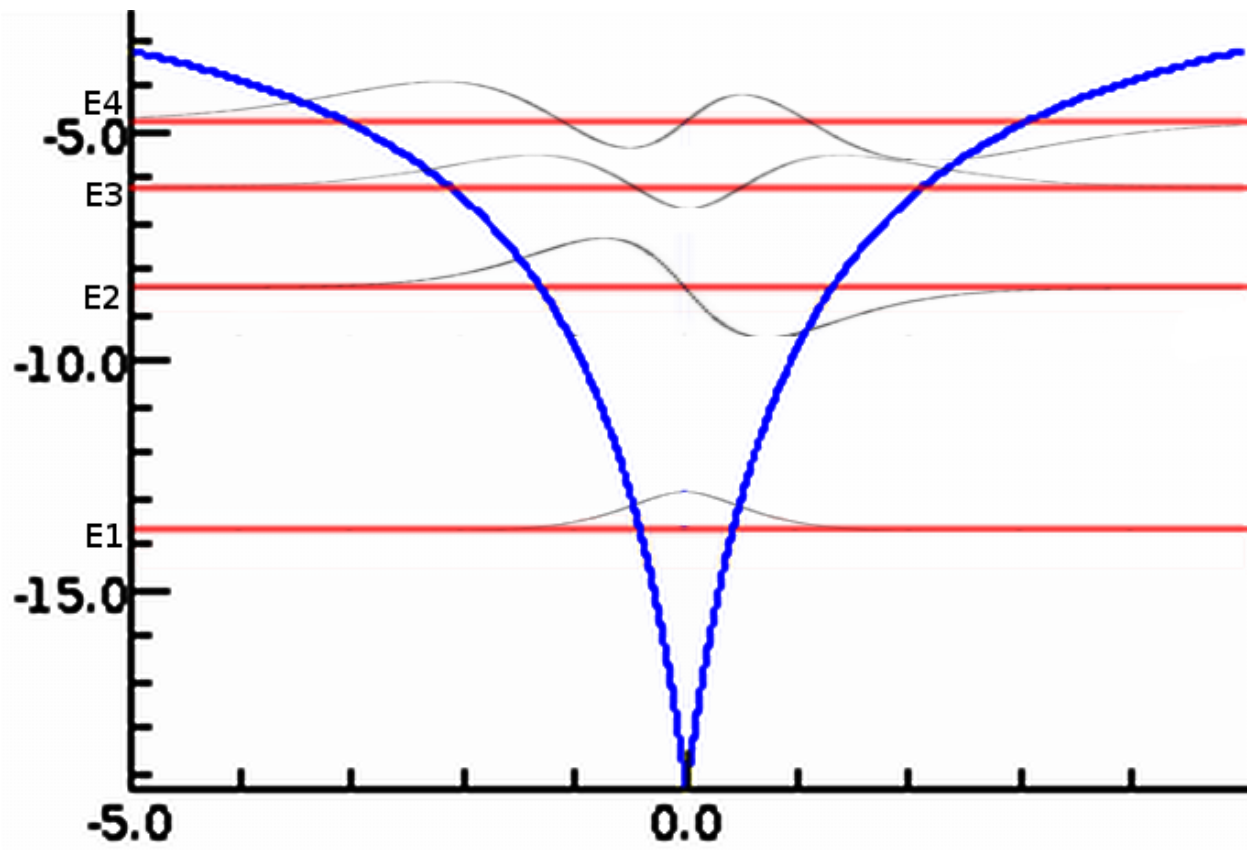


Figure 1: Energy levels and wave forms for $V = -19.4/(|x| + 1)$

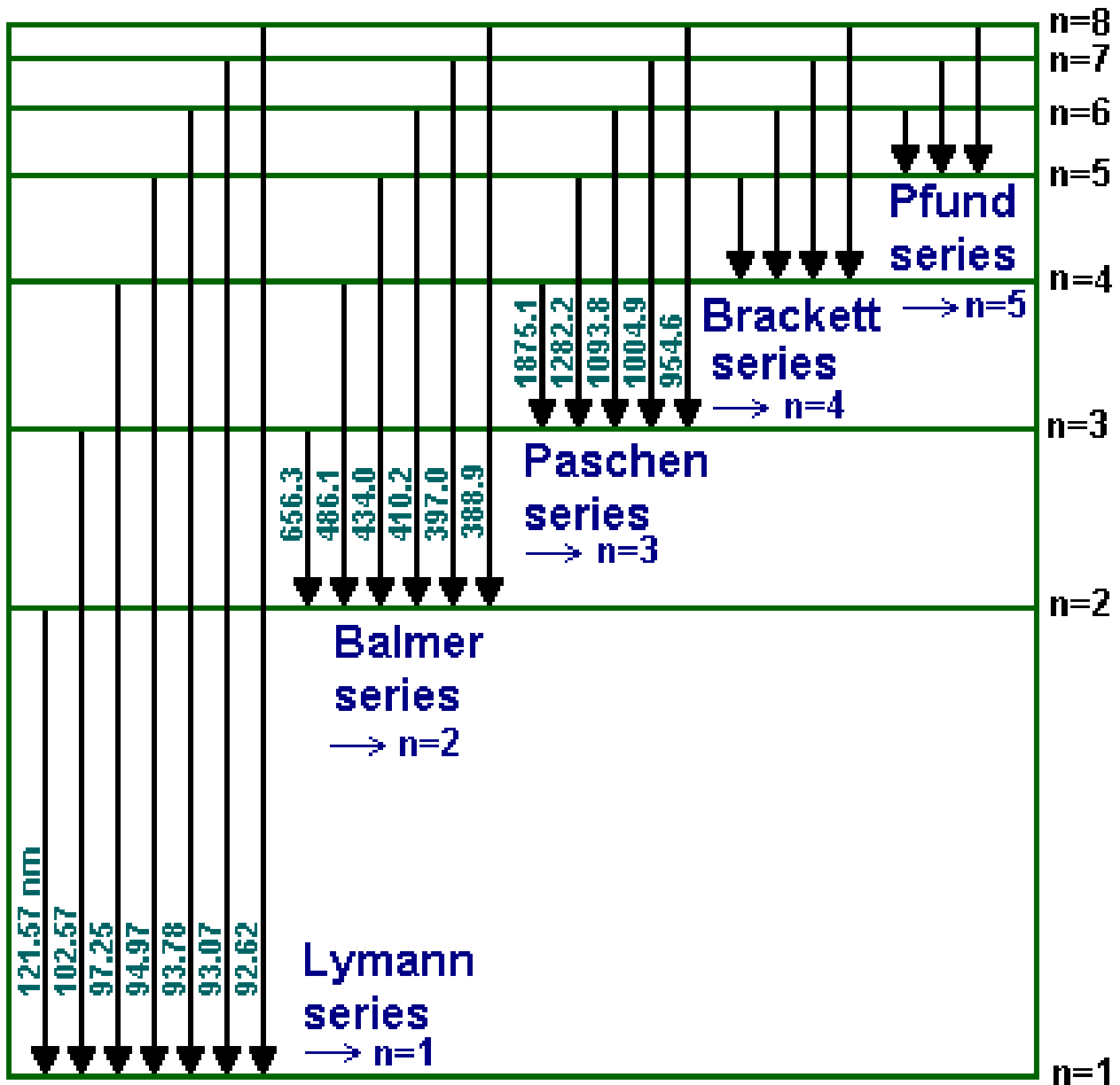


Figure 2: Energy spectrum for the hydrogen atom

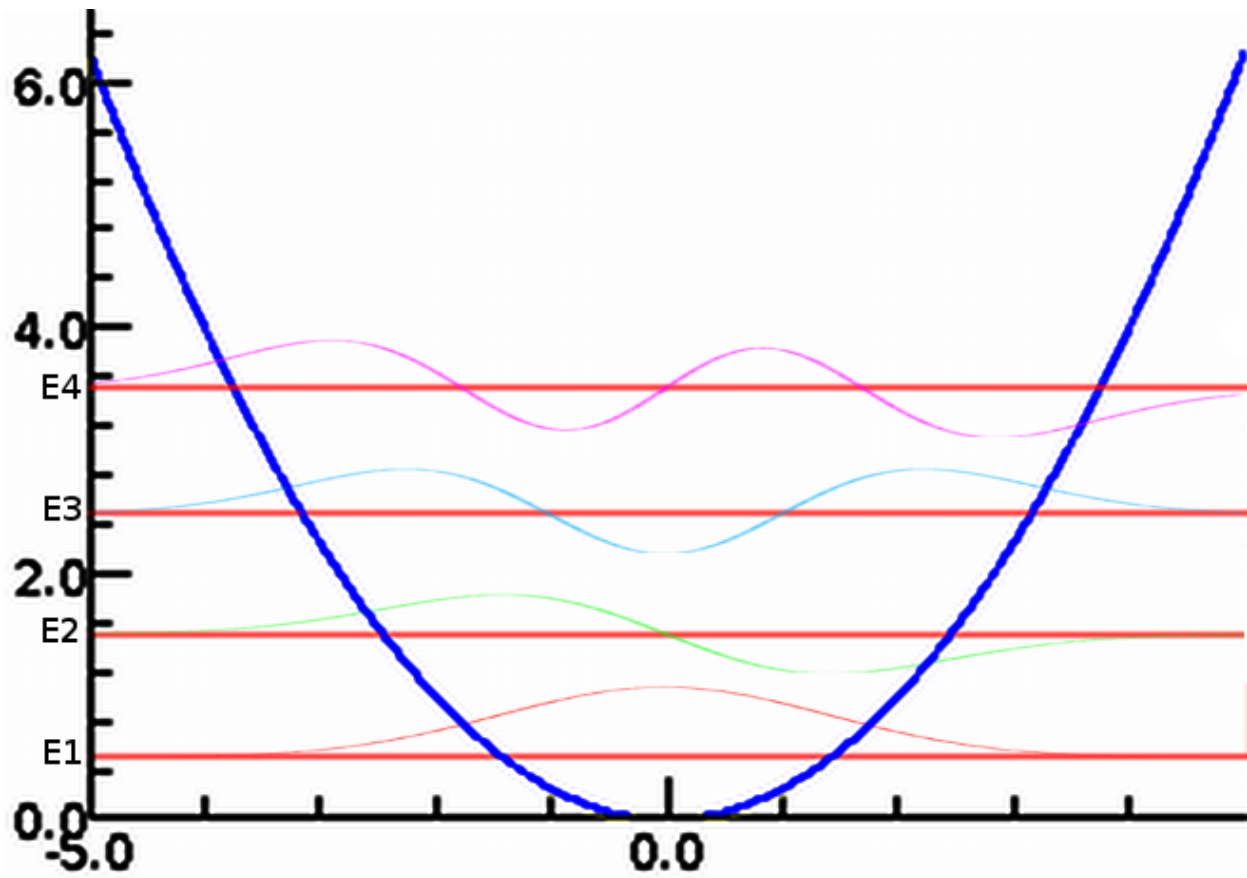


Figure 3: Energy levels and wave forms for $V = -19.4/(|x| + 1)$

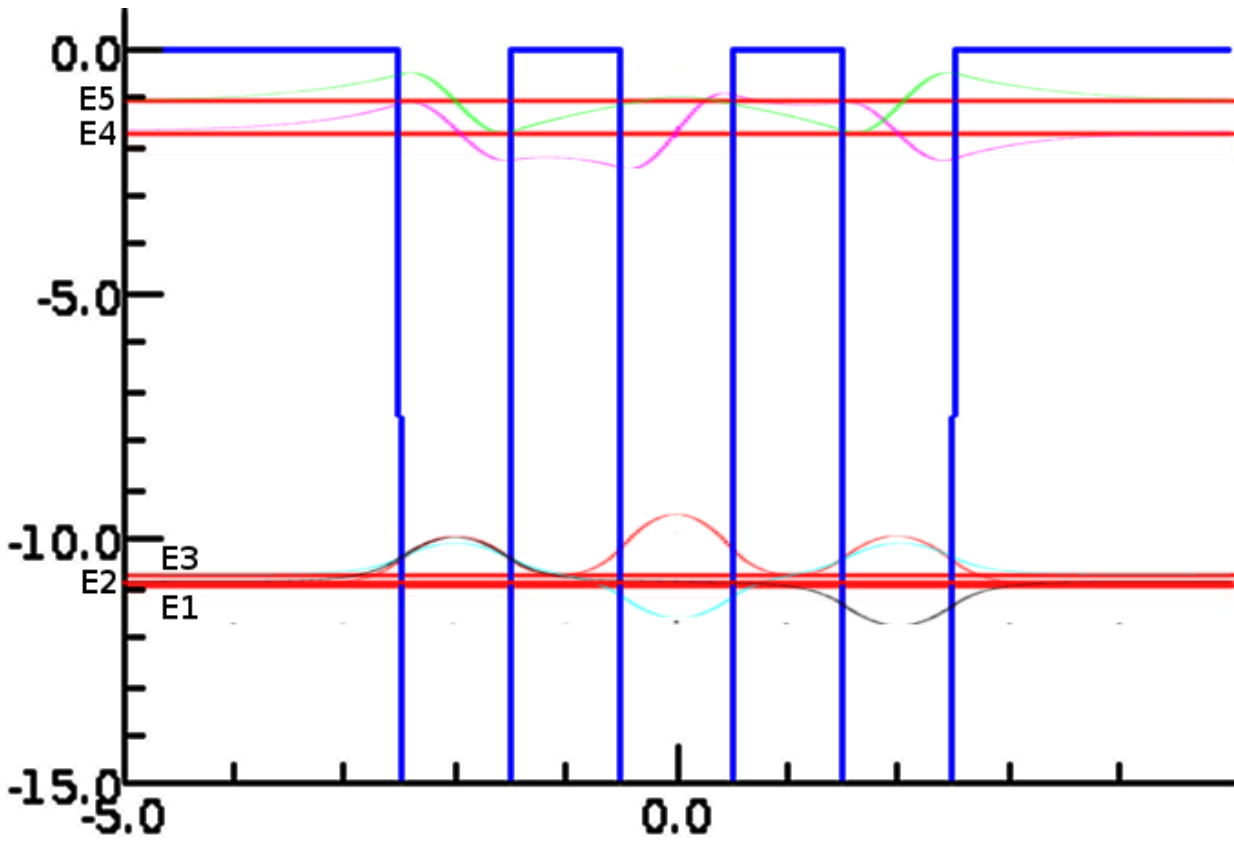


Figure 4: Energy levels and wave forms for $V = -19.4/(|x| + 1)$

$B \cos(kx)$ can be eliminated as a solution by using $\psi(0) = 0 = B \cos(k0) = B$. Using the boundary condition at $x = a$, we have $\psi(a) = 0 = A \sin ka$, or $ka = n\pi$, $n \in \mathbb{N}^*$, which gives $k = \frac{n\pi}{a}$. We can finally find A by normalizing the wave function:

$$\begin{aligned} 1 &= \int_0^a A^2 \sin^2\left(\frac{n\pi x}{a}\right) dx \\ &= A^2 \int_0^a \frac{1}{2} \left(1 - \cos\left(2\frac{n\pi x}{a}\right)\right) dx \\ &= \frac{A^2}{2} \left(x - \frac{a}{2n\pi} \sin\left(2\frac{n\pi x}{a}\right)\right) \Big|_{x=0}^a \\ &= \frac{A^2}{2} \left(a - \frac{a}{2n\pi} \sin\left(2\frac{n\pi a}{a}\right) - 0\right) \\ &= \frac{A^2}{2} \left(a - \frac{a}{2n\pi} \sin(2n\pi)\right) \\ &= \frac{A^2}{2} \left(a - \frac{a}{2n\pi} (0)\right) \\ &= A^2 \frac{a}{2} \\ \frac{2}{a} &= A^2 \\ \sqrt{\frac{2}{a}} &= A \end{aligned}$$

So, for $\psi(x)$ we finally have that

$$\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$$

Plugging this back into the time independent Schrödinger equation, we get:

$$\begin{aligned} \frac{d^2}{dx^2} \left(\sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \right) &= -\frac{2mE}{\hbar^2} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \\ -\left(\frac{n\pi}{a}\right)^2 \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) &= -\frac{2mE}{\hbar^2} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \\ -\left(\frac{n\pi}{a}\right)^2 &= -\frac{2mE}{\hbar^2} \\ \frac{\hbar^2 n^2 \pi^2}{2ma^2} &= E_n \end{aligned}$$

Part b

Solve for a so that the $n = 2 \rightarrow 1$ transition has the same wavelength as hydrogen.

We have $E_{H2 \rightarrow H1} = \frac{2\pi\hbar c}{\lambda}$. The first transition for the hydrogen atom is at $\lambda = 121.57$ (see figure 2, and [Tipler & Lewellyn, p. 150]). So, we have $E_{H2 \rightarrow H1} = \frac{2\pi c \hbar}{121.57}$. The energy transition from E_2 to E_1 should result in energy equal to

$$\begin{aligned} E_2 - E_1 &= \frac{4\hbar^2 \pi^2}{2ma^2} - \frac{\hbar^2 \pi^2}{2ma^2} \\ &= \frac{3\hbar^2 \pi^2}{2ma^2} \end{aligned}$$

Setting this equal to $E_{H2 \rightarrow H1}$, we get:

$$\begin{aligned} \frac{2\pi c \hbar}{121.57} &= \frac{3\hbar^2 \pi^2}{2ma^2} \\ a^2 &= \frac{3(121.57) \hbar \pi}{4cm} \\ a &= \sqrt{\frac{3(121.57) \hbar \pi}{4cm}} \end{aligned}$$

With m the mass of the electron, we get $a = 0.333$ nm.

Part c

Compare the wavelength of the $n = 3 \rightarrow 1$ transition with hydrogen.

Using $E = \frac{2\pi\hbar c}{\lambda} = E_3 - E_1$, we have:

$$\begin{aligned} \frac{2\pi\hbar c}{\lambda} &= \frac{9\hbar^2 \pi^2}{2ma^2} - \frac{\hbar^2 \pi^2}{2ma^2} \\ \frac{2\pi\hbar c}{\lambda} &= \frac{4\hbar^2 \pi^2}{ma^2} \\ \frac{2\pi\hbar c m a^2}{4\hbar^2 \pi^2} &= \lambda \\ \frac{c m a^2}{2\hbar \pi} &= \lambda \end{aligned}$$

Using a from part (c), we have $\lambda = 45.589$ nm. The wavelength for the $3 \rightarrow 1$ transition for hydrogen is $\lambda = 102.57$ nm (see figure 2). These are not equal.

Part d

What is the ionization potential in the model?

Because $E \sim n^2$, as $n \rightarrow \infty$, $E \rightarrow \infty$. So, the ionization potential would be infinite energy.

Part e

What properties of the infinite square well make it a bad approximation of hydrogen?

Once a value for a has been chosen, only that energy level will match the actual hydrogen atom. The energy levels don't get closer together as n increases, and there is no ionization energy. It's just wrong!

Problem 3

Consider the nucleus of heavy hydrogen, the deuteron, which is a proton and a neutron bound by the strong nuclear force. Since the neutron and proton have about the same mass, the reduced mass is $m = m_p m_n / (m_p + m_n) \approx \frac{1}{2} m_p = 469 \text{ MeV}/c^2$. The binding energy $B = 2.225 \text{ MeV}$ has been measured from the energy of the gamma ray produced when a neutron captures on a proton. Approximate this system as a neutron of reduced mass m in a square well, as shown in Figure 5. The radius of the deuteron is $a = 2.14 \text{ fm}$.

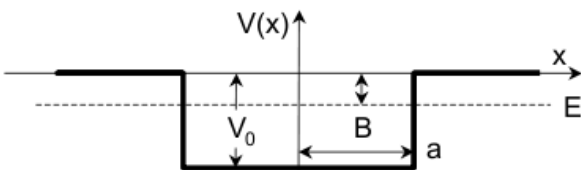


Figure 5: Square Well for a Reduced Mass Neutron

Part a

Use the wavefunctions $\psi_I(x) = A \cos(kx)$ inside the well, and $\psi_{II}(x) = e^{-\kappa|x|}$ outside. Show that these functions are solutions of the Schrödinger equation, and solve for k , κ as a function of V , B , a , m , and \hbar .

Using the time independent Schrödinger equation:

$$\frac{\hbar^2}{2m} \left(-i \frac{\partial}{\partial x} \right)^2 \psi(x) + V(x)\psi(x) = E\psi(x)$$

$$\left(-\frac{\hbar^2}{2m} \right) \frac{\partial^2}{\partial x^2} \psi(x) + V(x)\psi(x) = E\psi(x)$$

$$\left(-\frac{\hbar^2}{2m} \right) \frac{\partial^2}{\partial x^2} \psi(x) = E\psi(x) - V(x)\psi(x)$$

$$\left(-\frac{\hbar^2}{2m} \right) \frac{\partial^2}{\partial x^2} \psi(x) = \psi(x) (E - V(x))$$

we know that $\psi_I(x) = A \cos(kx)$ is a solution because:

$$-\frac{\partial^2}{\partial x^2} A \cos(kx) = A \cos(kx)$$

$$-A \frac{\partial^2}{\partial x^2} \cos(kx) = A \cos(kx)$$

$$k^2 \cos(kx) = \cos(kx)$$

And, if $k^2 = 1$, the differential equation is satisfied. Similarly, $\psi_{II}(x) = e^{-\kappa|x|}$ is a solution because:

$$\frac{\partial^2}{\partial x^2} e^{-\kappa|x|} = e^{-\kappa|x|}$$

$$\kappa^2 e^{-\kappa|x|} = e^{-\kappa|x|}$$

Here also, if $\kappa^2 = 1$, the differential equation is satisfied. Using these, we can calculate k and κ by substituting into Schrödinger's equation above:

$$\left(-\frac{\hbar^2}{2m} \right) \frac{\partial^2}{\partial x^2} A \cos(kx) = A \cos(kx) (E - V(x))$$

$$\frac{\hbar^2}{2m} k^2 \cos(kx) = \cos(kx) (E - V(x))$$

$$\frac{\hbar^2}{2m} k^2 = E - V(x)$$

Here, we have $V(x) = -V_0$, and $E = -B$. This gives:

$$\begin{aligned} k^2 &= \frac{2m(-B + V_0)}{\hbar^2} \\ k &= \sqrt{\frac{2m(-B + V_0)}{\hbar^2}} \\ &= \frac{\sqrt{2m(-B + V_0)}}{\hbar} \end{aligned}$$

Now, solving for κ :

$$\begin{aligned} \left(-\frac{\hbar^2}{2m}\right) \frac{\partial^2}{\partial x^2} e^{-\kappa|x|} &= e^{-\kappa|x|} (E - V(x)) \\ -\frac{\hbar^2}{2m} \kappa^2 e^{-\kappa|x|} &= e^{-\kappa|x|} (E - V(x)) \\ -\frac{\hbar^2}{2m} \kappa^2 &= E - V(x) \end{aligned}$$

Here, we have $V(x) = 0$, and $E = -B$. This gives:

$$\begin{aligned} -\kappa^2 &= \frac{-2Bm}{\hbar^2} \\ \kappa &= \sqrt{\frac{2Bm}{\hbar^2}} \\ &= \frac{\sqrt{2Bm}}{\hbar} \end{aligned}$$

Part b

Solve the two boundary conditions at $x = a$ to come up with the formula $\tan(ka) = \kappa a/ka$. Using the binding energy, calculate the value of κa and plot the LHS and RHS of the above equation as a function of ka . Circle the solutions for allowed values of ka , where the two curves cross. The lowest value represents the ground state. Using the value of ka from the crossing point, calculate the depth of the potential V and compare it to the binding energy of the hydrogen atom.

The two boundary conditions at $x = a$ are that $\psi_I(a) = \psi_{II}(a)$ and that $\psi'_I(a) = \psi'_{II}(a)$. Calculating ψ'_I and ψ'_{II} , we get:

$$\begin{aligned} \psi'_I(x) &= -Ak \sin(kx) \\ \psi'_{II}(x) &= -\kappa e^{-\kappa|x|} \end{aligned}$$

This gives us:

$$\begin{aligned} A \cos(ka) &= e^{-\kappa|a|} \\ -Ak \sin(ka) &= -\kappa e^{-\kappa|a|} \\ Ak \sin(ka) &= \kappa e^{-\kappa|a|} \end{aligned}$$

We can now divide the second result by the first to get:

$$\begin{aligned} \frac{Ak \sin(ka)}{A \cos(ka)} &= \frac{\kappa e^{-\kappa|a|}}{e^{-\kappa|a|}} \\ k \tan(ka) &= \kappa \\ \tan(ka) &= \frac{\kappa}{k} \\ \tan(ka) &= \frac{\kappa}{k} \left(\frac{a}{a}\right) \\ \tan(ka) &= \frac{\kappa a}{ka} \end{aligned}$$

Using the binding energy and other constants from above, we can calculate:

$$\begin{aligned} \kappa a &= \frac{\sqrt{2Bm}}{\hbar} a \\ &= \frac{\sqrt{2(2.225 \text{ MeV})(469 \text{ MeV})}}{\hbar c} (2.14 \text{ fm}) \\ &\approx 0.495 \end{aligned}$$

Now we can plot $f(ka) = \tan(ka)$ and $g(ka) = \frac{0.495}{ka}$. This gives us figure 6.

Estimating the lowest value ka crossing point to be at 0.6, we can calculate V using:

$$\begin{aligned} 0.6 &= \frac{\sqrt{2m(-B + V_0)}}{\hbar} a \\ \frac{1}{2m} \left(\frac{0.6 \hbar}{a}\right)^2 + B &= V_0 \end{aligned}$$

This gives $V_0 = \frac{c^2}{2(469 \text{ MeV})} \left(\frac{0.6 \hbar}{2.14 \text{ fm}}\right)^2 + 2.225 \text{ MeV}$, or $V_0 \approx 5.49 \text{ MeV}$. This is much greater than the binding energy of the hydrogen atom.

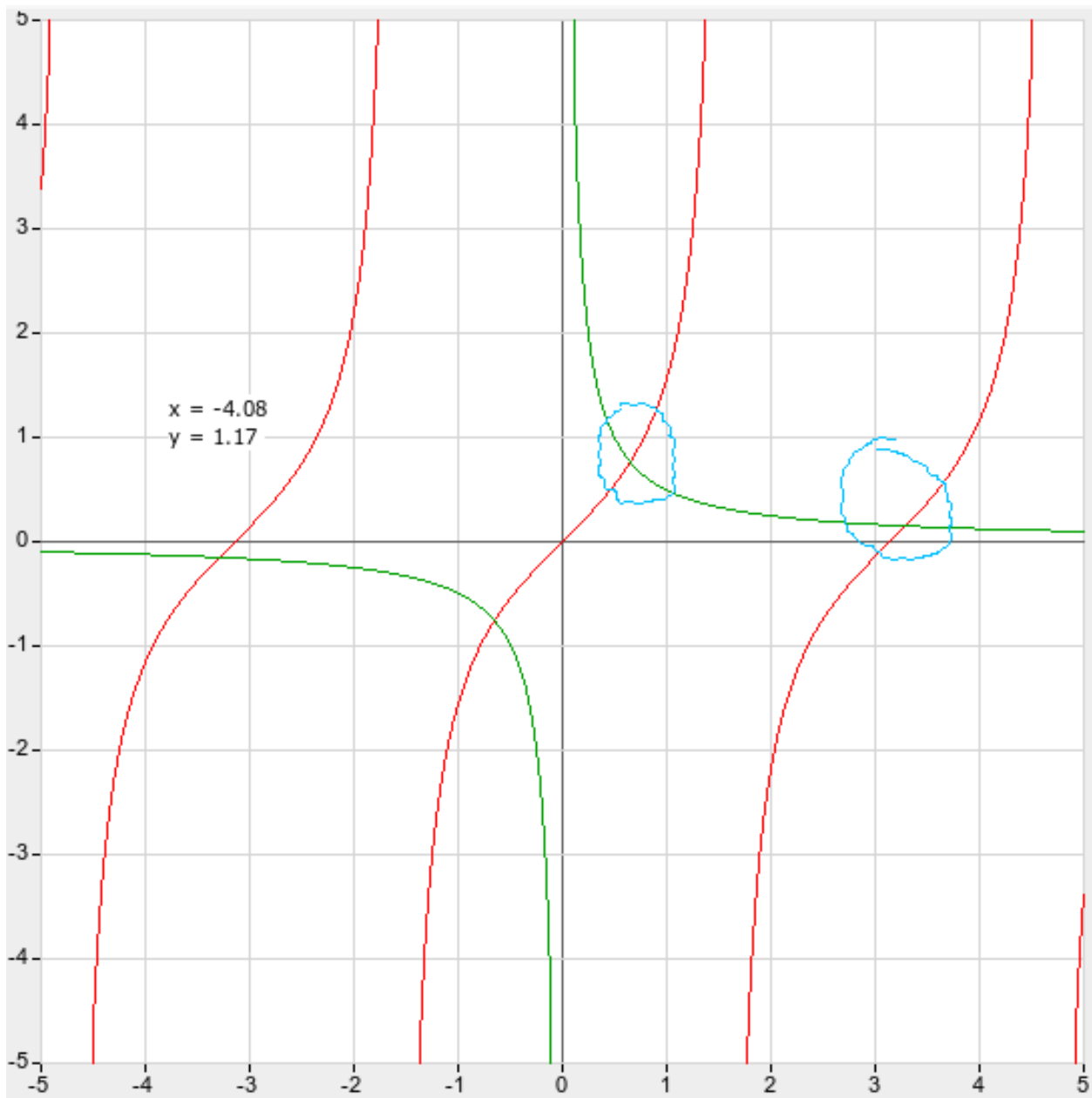


Figure 6: Plot of $f(ka) = \tan(ka)$ and $g(ka) = \frac{0.495}{ka}$ with intersection points circled

Part c

Are there any excited states of the deuteron?
Hint: compare the energy of the first excited state to V (no calculation necessary).

No. The first "excited state" will completely free the pairing.

Problem 4

Consider the step potential

$$V(x) = V_0 \cdot \theta(x) = \begin{cases} 0 & \text{in region 1 } (x < 0) \\ V_0 & \text{in region 2 } (x > 0) \end{cases}$$

Part a

What type of force does this potential describe?

This potential represents an impulse.

Part b

Show that $\psi(x) = e^{\pm ik_i x}$ are solutions of the Schrödinger equation for this potential in region 1 ($x < 0$) and region 2 ($x > 0$).

The time independent Schrödinger's equation is:

$$\frac{\hbar^2}{2m} \left(-i \frac{\partial}{\partial x} \right)^2 \psi(x) + V(x)\psi(x) = E\psi(x)$$

In region 1, this becomes:

$$\frac{\hbar^2}{2m} \left(-i \frac{\partial}{\partial x} \right)^2 \psi(x) = E\psi(x)$$

And in region 2 this becomes:

$$\frac{\hbar^2}{2m} \left(-i \frac{\partial}{\partial x} \right)^2 \psi(x) = \psi(x) (E - V_0)$$

Substituting in $\psi(x) = e^{\pm ik_i x}$ into these equations yields, for the $V(x) = 0$ region:

$$\begin{aligned} \left(-\frac{\hbar^2}{2m} \right) \frac{\partial^2}{\partial x^2} e^{\pm ik_1 x} &= E e^{\pm ik_1 x} \\ \left(-\frac{\hbar^2}{2m} \right) (\pm i)^2 k_1^2 e^{\pm ik_1 x} &= E e^{\pm ik_1 x} \\ \left(\frac{\hbar^2}{2m} \right) k_1^2 e^{\pm ik_1 x} &= E e^{\pm ik_1 x} \end{aligned}$$

Since $e^{\pm ik_i x}$ cancels, this is a solution to the $V(x) = 0$ region. For the $V(x) = V_0$ region, we have:

$$\begin{aligned} \left(-\frac{\hbar^2}{2m} \right) \frac{\partial^2}{\partial x^2} e^{\pm ik_2 x} &= e^{\pm ik_2 x} (E - V_0) \\ \left(-\frac{\hbar^2}{2m} \right) (\pm i)^2 k_2^2 e^{\pm ik_2 x} &= e^{\pm ik_2 x} (E - V_0) \\ \left(\frac{\hbar^2}{2m} \right) k_2^2 e^{\pm ik_2 x} &= e^{\pm ik_2 x} (E - V_0) \end{aligned}$$

Once again, $e^{\pm ik_i x}$ cancels, so this is a solution to the time-independent Schrödinger's equation.

Part c

Calculate k_i in regions $i = 1, 2$ in terms of the total energy E .

In region 1, we have:

$$\begin{aligned} \left(-\frac{\hbar^2}{2m} \right) (\pm i)^2 k_1^2 e^{\pm ik_1 x} &= E e^{\pm ik_1 x} \\ \left(\frac{\hbar^2}{2m} \right) k_1^2 e^{\pm ik_1 x} &= E e^{\pm ik_1 x} \\ \left(\frac{\hbar^2}{2m} \right) k_1^2 &= E \\ k_1^2 &= \frac{2mE}{\hbar^2} \\ k_1 &= \pm \sqrt{\frac{2mE}{\hbar^2}} \\ k_1 &= \pm \frac{\sqrt{2mE}}{\hbar} \end{aligned}$$

In region 2, we have:

$$\left(-\frac{\hbar^2}{2m}\right)(\pm i)^2 k_2^2 e^{\pm ik_2 x} = e^{\pm ik_2 x} (E - V_0)$$

$$\left(\frac{\hbar^2}{2m}\right) k_2^2 e^{\pm ik_2 x} = e^{\pm ik_2 x} (E - V_0)$$

$$\left(\frac{\hbar^2}{2m}\right) k_2^2 = (E - V_0)$$

$$k_2^2 = \frac{2m(E - V_0)}{\hbar^2}$$

$$k_2 = \pm \frac{\sqrt{2m(E - V_0)}}{\hbar}$$

Part d

To describe the reflection and transmission of a quantum particle, let the total wavefunction be $\psi(x) = Ae^{ik_1 x} + Be^{-ik_1 x}$ if $x < 0$ and $\psi(x) = Ce^{ik_2 x}$ if $x > 0$. Label the incident, transmitted, and reflected wave functions. Why is the term $De^{-ik_2 x}$ not included?

$Ae^{ik_1 x}$ is the incident wave function. $Be^{-ik_1 x}$ is the reflected wave function. $Ce^{ik_2 x}$ is the transmitted wave function. $De^{-ik_2 x}$ is not included because it describes a wave incident from the right, but nothing comes from the right (that is, there is no causality for this term), so this term must go to zero.

Part e

Apply the boundary conditions at $x = 0$ to obtain formulas for the coefficients of reflections $R \equiv \left(\frac{B}{A}\right)^2$ and transmission $T \equiv \frac{k_2}{k_1} \left(\frac{C}{A}\right)^2$ as a function of E/V_0 (the factor of k_2/k_1 accounts for the difference in velocity).

If $\psi_1(x) = Ae^{ik_1 x} + Be^{-ik_1 x}$ and $\psi_2(x) = Ce^{ik_2 x}$, then at the boundary conditions we have that $\psi_1(0) = \psi_2(0)$, and that $\psi_1'(0) = \psi_2'(0)$. Calculating the first derivatives, so that we can relate these boundary conditions, we get:

$$\psi_1'(x) = ik_1 Ae^{ik_1 x} - ik_1 Be^{-ik_1 x}$$

$$\psi_2'(x) = ik_2 Ce^{ik_2 x}$$

So, at the boundary conditions we get:

$$\psi_1(0) = \psi_2(0)$$

$$Ae^{ik_1(0)} + Be^{-ik_1(0)} = Ce^{ik_2(0)}$$

$$A + B = C$$

and:

$$\psi_1'(0) = \psi_2'(0)$$

$$ik_1 Ae^{ik_1(0)} - ik_1 Be^{-ik_1(0)} = ik_2 Ce^{ik_2(0)}$$

$$k_1 A - k_1 B = k_2 C$$

To find $R = \left(\frac{B}{A}\right)^2$, we can multiply $A + B = C$ through by k_2 and then subtract $k_1 A - k_1 B = k_2 C$:

$$\begin{array}{r} k_2 A + k_2 B = k_2 C \\ (-) \quad k_1 A - k_1 B = k_2 C \\ \hline (k_2 - k_1) A + (k_2 + k_1) B = 0 \end{array}$$

So, $-(k_2 - k_1)A = (k_2 + k_1)B$, or $\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2}$, and $R = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$. Similarly, to find $T = \frac{k_2}{k_1} \left(\frac{C}{A}\right)^2$ we can multiply $A + B = C$ through by k_1 and add $k_1 A - k_1 B = k_2 C$. This yields:

$$\begin{array}{r} k_1 A + k_1 B = k_1 C \\ (+) \quad k_1 A - k_1 B = k_2 C \\ \hline 2k_1 A + 0 = (k_1 + k_2) C \end{array}$$

So, $\frac{C}{A} = \frac{2k_1}{(k_1 + k_2)}$, and $T = \frac{k_2}{k_1} \left(\frac{2k_1}{(k_1 + k_2)}\right)^2 = \frac{4k_1 k_2}{(k_1 + k_2)^2}$. Choosing positive k_1 and k_2 and substituting in $k_1 = \frac{\sqrt{2mE}}{\hbar}$ and $k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar}$ we get:

$$\begin{aligned} R &= \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 \\ &= \left(\frac{\frac{\sqrt{2mE}}{\hbar} - \frac{\sqrt{2m(E - V_0)}}{\hbar}}{\frac{\sqrt{2mE}}{\hbar} + \frac{\sqrt{2m(E - V_0)}}{\hbar}}\right)^2 \\ &= \left(\frac{(\sqrt{E} - \sqrt{E - V_0})}{(\sqrt{E} + \sqrt{E - V_0})}\right)^2 \end{aligned}$$

ergy $\hbar^2/2mL^2$, where L is some length.

and:

$$\begin{aligned} T &= \frac{4k_1k_2}{(k_1+k_2)^2} \\ &= \frac{4\left(\frac{\sqrt{2mE}}{\hbar}\right)\left(\frac{\sqrt{2m(E-V_0)}}{\hbar}\right)}{\left(\frac{\sqrt{2mE}}{\hbar} + \frac{\sqrt{2m(E-V_0)}}{\hbar}\right)^2} \\ &= \frac{4\frac{2m}{\hbar^2}(\sqrt{E^2-EV_0})}{\left(\frac{\sqrt{2m}}{\hbar}\left(\sqrt{E} + \sqrt{(E-V_0)}\right)\right)^2} \\ &= \frac{4\frac{2m}{\hbar^2}(\sqrt{E^2-EV_0})}{\frac{2m}{\hbar^2}\left(\sqrt{E} + \sqrt{(E-V_0)}\right)^2} \\ &= \frac{4(\sqrt{E^2-EV_0})}{\left(\sqrt{E} + \sqrt{(E-V_0)}\right)^2} \end{aligned}$$

Part f

Show that $R+T=1$, i.e. the particle is either reflected or transmitted.

Using $R = \left(\frac{k_1-k_2}{k_1+k_2}\right)^2$ and $T = \frac{4k_1k_2}{(k_1+k_2)^2}$, we get:

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

Problem 6.3

In a region of space, a particle has a wave function given by $\psi(x) = Ae^{-x^2/2L^2}$ and en-

Part a

Find the potential energy as a function of x , and sketch V versus x .

We start with the time-independent Schrödinger equation:

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

Since we know $\psi(x)$ and E , it is possible to determine $V(x)$, the potential energy:

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

Substituting in for $\psi(x)$ and E , we have:

$$\begin{aligned} V(x) &= \frac{\hbar^2}{2mL^2} + \frac{\hbar^2}{2mAe^{-x^2/2L^2}} \frac{d^2Ae^{-x^2/2L^2}}{dx^2} \\ &= \frac{\hbar^2}{2mL^2} + \frac{\hbar^2}{2mAe^{-x^2/2L^2}} \frac{d\left(\frac{-x}{L^2}e^{-x^2/2L^2}\right)}{dx} \\ &= \frac{\hbar^2}{2mL^2} \left(1 + \frac{\frac{d}{dx}\left(-xe^{-x^2/2L^2}\right)}{e^{-x^2/2L^2}}\right) \\ &= \frac{\hbar^2}{2mL^2} \left(1 + \frac{-e^{-x^2/2L^2} + \frac{x^2}{L^2}e^{-x^2/2L^2}}{e^{-x^2/2L^2}}\right) \\ &= \frac{\hbar^2}{2mL^2} \left(1 - 1 + \frac{x^2}{L^2}\right) \\ &= \frac{\hbar^2 x^2}{2mL^4} \end{aligned}$$

The graph of the potential is shown in figure 7.

Part b

What is the classical potential that has this dependence?

Since \hbar^2/mL^4 is just a constant, we can call it k , in which case $V(x) = \frac{1}{2}kx^2$. This is the potential for a simple harmonic oscillator.

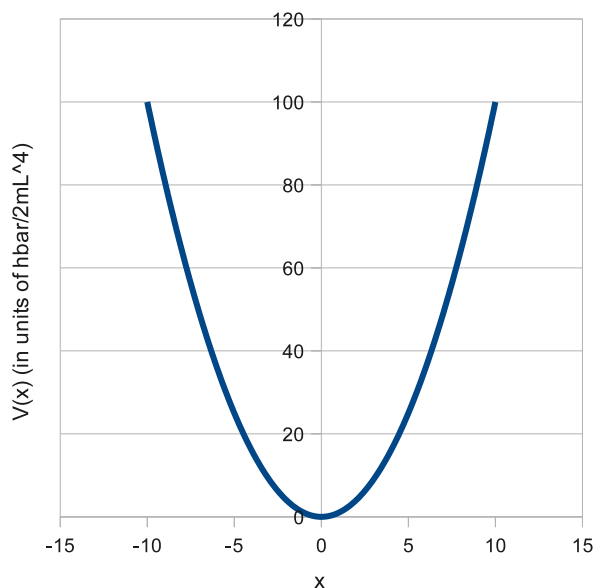


Figure 7: Graph of $V(x) = \frac{\hbar^2 x^2}{2mL^4}$

Problem 6.4

Part a

For problem 6.3, find the kinetic energy as a function of x .

We know that $E = T + V$, so $T = E - V$. This gives us

$$\begin{aligned} T &= \frac{\hbar^2}{2mL^2} - \frac{\hbar^2 x^2}{2mL^4} \\ &= \frac{\hbar^2}{2mL^2} \left(1 - \frac{x^2}{L^2} \right) \end{aligned}$$

Part b

Show that $x = L$ is the classical turning point.

From our equation for T , $T = \frac{\hbar^2}{2mL^2} \left(1 - \frac{x^2}{L^2} \right)$, we see that at $x = L$, we have $T = \frac{\hbar^2}{2mL^2} \left(1 - \frac{L^2}{L^2} \right) = 0$.

Algorithm 0.1 Equation 6-21 from the book

$$\begin{aligned} V(x) &= 0 & 0 < x < L \\ V(x) &= \infty & x < 0 \text{ and } x > L \end{aligned}$$

Classical turning points occur when the kinetic energy is zero, which in this case occurs at $x = L$.

Part c

The potential energy of a simple harmonic oscillator in terms of its angular frequency ω is given by $V(x) = \frac{1}{2}m\omega^2 x^2$. Compare this with your answer to part (a) of problem 6.3, and show that the total energy for this wave function can be written $E = \frac{1}{2}\hbar\omega$.

In part (a) of problem 6.3, we have that $V(x) = \frac{\hbar^2 x^2}{2mL^4}$. This equation can be modified to better resemble $V(x) = \frac{1}{2}m\omega^2 x^2$ by:

$$\begin{aligned} V(x) &= \frac{\hbar^2 x^2}{2mL^4} \\ &= \frac{1}{2}m\omega^2 \cdot \frac{\hbar^2}{m^2 L^4} \end{aligned}$$

This gives $\omega = \frac{\hbar}{mL^2}$. We can now see that:

$$\begin{aligned} E &= \frac{1}{2}\hbar \cdot \frac{\hbar}{mL^2} \\ &= \frac{1}{2}\hbar\omega \end{aligned}$$

Problem 6.10

A particle is in the ground state of an infinite square well potential given by Equation 6-21. Find the probability of finding the particle in the interval $\Delta x = 0.002L$ at the following values for x (note that since Δx is very small, you need not do any integration).

Part a

$$x = L/2$$

From problem 2, we have $\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$. In the ground state, with $n = 1$, we have $\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right)$. Substituting in $x = L/2$, we get:

$$\begin{aligned}\psi(x) &= \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{2}\right) \\ &= \sqrt{\frac{2}{L}}\end{aligned}$$

Using the mandated approximation, the probability is given by $|\psi(x)|^2 \Delta x$, or $\frac{2}{L} \cdot 0.002 L = 0.004$

Part b

$$x = 2L/3$$

From problem 2, we have $\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$. In the ground state, with $n = 1$, we have $\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right)$. Substituting in $x = 2L/3$, we get:

$$\begin{aligned}\psi(x) &= \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi}{3}\right) \\ &= \sqrt{\frac{2}{L}} \sqrt{\frac{3}{4}} \\ &= \sqrt{\frac{3}{2L}}\end{aligned}$$

The probability is given by $|\psi(x)|^2 \Delta x$, or $\frac{3}{2L} \cdot 0.002 L = 0.003$

Part c

$$x = L$$

This one is trickier. Since $\psi(L) = 0$, but $\Delta x \neq 0$, we can't actually calculate the function at $\psi(L)$. Instead, we can recognize that half the width of Δx , outside the well, has zero probability, and so will not contribute to the total probability. Instead, we can look at the remaining half of the interval, Δx , inside the well. This has a width of $\Delta x/2 = 0.001 L$, and should be evaluated at $x = L(1 - 0.001/2)$. From $\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right)$, we get:

$$\begin{aligned}\psi(x) &= \sqrt{\frac{2}{L}} \sin(\pi(1 - 0.001/2)) \\ &= \sqrt{\frac{2}{L}} (0.00157)\end{aligned}$$

The probability is given by $|\psi(x)|^2 \Delta x$, or:

$$\frac{2}{L} (0.00157)^2 \cdot 0.001 L \approx 4.9348 \times 10^{-9}$$

Or, $|\psi(x)|^2 \Delta x \approx 0$. Incidentally, naively calculating at $x = L$ also gives $|\psi(x)|^2 \Delta x = 0$, which is probably sufficient as an approximation in this case.