Physics 70007, Fall 2009
Solutions to HW #5

December 2, 2009

1. Consider the case of a particle with mass $m$ in an infinite potential well defined by a potential $V(x) = 0$ for $0 \leq x \leq L$ and $V(x) = \infty$ otherwise.

(a) Find the eigenfunctions $\psi_n(x)$ and the energy spectrum $E_n$.

Outside the well, the wavefunction is forced to be zero due to the infinite potential; at the boundaries of the well, $\psi$ must be continuous, but $\psi'$ need not be, because of the infinite discontinuity in the potential. The continuity of $\psi$ gives us the boundary conditions $\psi(0) = \psi(L) = 0$.

Inside the well, the potential is zero, so the Schrödinger equation takes the form

$$-\frac{\hbar^2}{2m} \psi'' = E\psi \quad \rightarrow \quad \psi'' + \frac{2mE}{\hbar^2} \psi = 0$$

The solutions of the differential equation (within the well) take the form

$$\psi(x) = A \cos \left( x \sqrt{\frac{2mE}{\hbar^2}} \right) + B \sin \left( x \sqrt{\frac{2mE}{\hbar^2}} \right)$$

where $A$ and $B$ are constants. Applying the boundary condition at $x = 0$ forces $A$ to be zero; then applying the other boundary condition leads to quantization of the possible energies of the particle:

$$B \sin \left( L \sqrt{\frac{2mE}{\hbar^2}} \right) = 0 \quad \rightarrow \quad L \sqrt{\frac{2mE_n}{\hbar^2}} = n\pi$$

where $n$ is an positive integer (if $n$ is zero, then $\psi$ becomes identically zero; negative $n$ gives us nothing new compared to positive $n$). Solving for $E_n$:

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

Using the quantization condition, we can rewrite the eigenfunctions in a simple form:

$$\psi_n(x) = B_n \sin \left( \frac{n\pi x}{L} \right)$$

The normalization integral fixes $B_n$:

$$1 = \int_0^L dx \, |B_n|^2 \sin^2 \left( \frac{n\pi x}{L} \right) = |B_n|^2 \cdot \frac{L}{2}$$

Choosing $B_n$ to be real and positive, we have at last

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \left( \frac{n\pi x}{L} \right)$$
(b) Sketch (not to scale, but to show all important features) the wave function and the probability density for the ground state and the first two excited states (i.e. for \( n = 1, 2, 3 \)).

Let us plot \( \psi_n \) (as found in part a) and \( |\psi_n|^2 = \frac{2}{L} \sin^2 \left( \frac{n\pi x}{L} \right) \) for \( n = 1, 2, 3 \):

One important feature to note is the number of nodes (i.e. places where \( \psi = 0 \)) inside the well: for a given state \( n \), there are \((n-1)\) nodes, occurring at locations \( x = L \cdot \frac{a}{n}, a = 1, 2, \ldots, n-1 \). Another thing to notice about the solutions is their parity (defined with respect to the center of the well, which is located at \( x = \frac{L}{2} \)). In general, the solutions with odd \( n \) have even parity (i.e. they satisfy \( \psi \left( \frac{L}{2} + x \right) = \psi \left( \frac{L}{2} - x \right) \)), and vice versa.

(c) What is the probability of finding the particle between \( x = 0 \) and \( x = L/n \) provided that the particle is in the \( n = 3 \) excited state? Generalize your result for arbitrary \( n \).

We can do this calculation directly for arbitrary \( n \), by integrating the probability density:

\[
\text{prob} = \int_0^{L/n} dx \ |\psi_n (x)|^2 \\
= \int_0^{\pi} dx \ \frac{2}{L} \sin^2 \left( \frac{n\pi x}{L} \right) \\
= \frac{2}{n\pi} \int_0^{\pi} dw \ \sin^2 w \ \left( w \equiv \frac{n\pi x}{L} \right) \\
= \frac{2}{n\pi} \cdot \frac{\pi}{2} \\
= \frac{1}{n}
\]

(where we “did” the integral by remembering that the average value of \( \sin^2 w \) over a full cycle is \( 1/2 \)). In particular, for \( n = 3 \) we get a probability of \( 1/3 \).

This result becomes more obvious once we realize from our work in part (b) that \( x = L/n \) is the location of the first node, so we are asking for the probability of finding the particle between the wall and the first node. But \( \psi_n \) has \( n - 1 \) nodes, which divide up the full extent of the well into \( n \) regions, and the particle is equally likely to be found in any one of those regions; so the probability for any one region should be \( 1/n \).

(d) Estimate the quantum number \( n \) of an electron with energy \( E = 30 \ eV \) trapped in a one dimensional potential well of width \( L = 1 \ \AA \). What is the typical quantum number \( n \) if a \( ^4 \text{He} \) atom is trapped instead of an electron? (Keep the energy at \( E = 30 \ eV \) for the \( ^4 \text{He} \) as well).
We use the energy quantization condition from part (a), in the form

\[ L \frac{2 (mc^2) E_n}{\pi} = n \]

where we have solved for \( n \), and inserted factors of \( c \) strategically so that we can use \( hc \approx 200 \text{ eV nm} \). For the electron, we have \( mc^2 \approx 511 \times 10^3 \text{ eV} \), and taking \( E = 30 \text{ eV} \) and \( L = 1 \text{ Å} = 0.1 \text{ nm} \), we find

\[ n = 0.88 \approx 1 \]

For the helium atom, we have \( mc^2 \approx 4 \times 939 \times 10^6 \text{ eV} \), with everything else the same; we find \( n \approx 75 \).

2. Let us now consider the behavior of a particle with the same mass \( m \) but now in a finite potential well: \( V(x) = 0 \) for \(-L \leq x \leq L\) and \( V(x) = V_0\) otherwise.

(a) Find the eigenfunctions \( \psi_n(x) \) and the equation for the energy spectrum \( E_n \), for the states bound in this potential well. Show that the equation for \( E_n \) takes the following form:

\[ (K^2 - 2\xi^2) \sin (2\xi) + 2\xi \sqrt{K^2 - \xi^2} \cos (2\xi) = 0 \]

where \( K^2 \equiv (2mV_0L^2)/\hbar^2 \) and \( \xi \equiv L\sqrt{2mE/\hbar^2} \). Show that this equation can be recast into the form

\[ \xi + \sin^{-1}(\xi/K) = \frac{n\pi}{2} \]

[where \( n \) is required to be an integer].

First note that we are considering bound states in the well; these states have energies satisfying \( 0 < E < V_0 \). Outside the well, even though the energy is less than the potential, the particle still has a finite probability to be found there! (In problem 1, the potential outside the well was infinite, which forced the wavefunction & hence the probability to zero in those regions.)

The well divides space into 3 regions: \( x \leq -L \), \( -L \leq x \leq L \), and \( x \geq L \). Our strategy will be to write down the solution in each region, and then patch these solutions together using our knowledge that \( \psi \) and \( \psi' \) must be continuous even at the boundaries between regions.

In the classically forbidden region outside the well, the solutions to the Schrödinger equation are linear combinations of exponentials \( \exp \left( \pm x \cdot \sqrt{2m(V_0 - E)/\hbar^2} \right) = \exp \left( \pm x \cdot \sqrt{K^2 - \xi^2}/L \right) \). For each region outside the well, one of the exponentials will go to zero for large \( |x| \) and will be normalizable, while the other exponential will go to infinity and so cannot be normalized. The coefficient of the non-normalizable exponential is forced to be zero.

Inside the well, the solutions will be linear combinations of exponentials with imaginary exponents, or equivalently sines and cosines: \( \sin \left( x \cdot \sqrt{2mE/\hbar^2} \right) = \sin (x \cdot \xi/L) \) and \( \cos \left( x \cdot \sqrt{2mE/\hbar^2} \right) = \cos (x \cdot \xi/L) \). There is no intrinsic reason to rule out either solution, so in general we must keep them both (although it will turn out that each eigenstate will be purely one or the other, because non-degenerate eigenstates must have definite parity whenever the Hamiltonian is parity-invariant).

We can summarize our general solution as

\[ \psi(x) = \begin{cases} 
A \exp \left( \frac{\sqrt{K^2 - \xi^2}}{L} x \right) & \text{for } x \leq -L \\
B \sin \left( \frac{\xi}{L} x \right) + C \cos \left( \frac{\xi}{L} x \right) & \text{for } -L \leq x \leq L \\
D \exp \left( -\frac{\sqrt{K^2 - \xi^2}}{L} x \right) & \text{for } x \geq L 
\end{cases} \]
where \( A, B, C, D \) are constants which we now proceed to determine from the matching conditions.

From continuity of \( \psi \) at \( x = -L \) we obtain

\[
A \exp \left( \frac{\sqrt{K^2 - \xi^2}}{L} (-L) \right) = B \sin \left( \frac{\xi}{L} (-L) \right) + C \cos \left( \frac{\xi}{L} (-L) \right)
\]

or

\[
A \exp \left( -\sqrt{K^2 - \xi^2} \right) = -B \sin \xi + C \cos \xi
\]

using the properties of \( \sin \) and \( \cos \) under parity. Similarly from continuity of \( \psi \) at \( x = L \) we find

\[
D \exp \left( -\sqrt{K^2 - \xi^2} \right) = B \sin \xi + C \cos \xi
\]

Now from continuity of \( \psi' \) at \( x = -L \) we obtain

\[
\frac{\sqrt{K^2 - \xi^2}}{L} \cdot A \exp \left( \frac{\sqrt{K^2 - \xi^2}}{L} (-L) \right) = \frac{\xi}{L} \cdot B \cos \left( \frac{\xi}{L} (-L) \right) + \frac{\xi}{L} \cdot -C \sin \left( \frac{\xi}{L} (-L) \right)
\]

or

\[
\frac{\sqrt{K^2 - \xi^2}}{\xi} \cdot A \exp \left( -\sqrt{K^2 - \xi^2} \right) = B \cos \xi + C \sin \xi
\]

while from continuity of \( \psi' \) at \( x = L \) we find

\[
-\frac{\sqrt{K^2 - \xi^2}}{\xi} \cdot D \exp \left( -\sqrt{K^2 - \xi^2} \right) = B \cos \xi - C \sin \xi
\]

We have thus found four equations for our four unknown constants \( A, B, C, D \). If we change \( A, D \) to \( A' \equiv A \exp \left( -\sqrt{K^2 - \xi^2} \right) \) and \( D' \equiv D \exp \left( -\sqrt{K^2 - \xi^2} \right) \), then we can write our equations in matrix form as

\[
\begin{pmatrix}
-1 & -\sin \xi & \cos \xi & 0 \\
0 & \sin \xi & \cos \xi & -1 \\
-\frac{\sqrt{K^2 - \xi^2}}{\xi} \cdot \cos \xi & \sin \xi & 0 \\
0 & \cos \xi & -\sin \xi & \sqrt{\frac{K^2 - \xi^2}{\xi}}
\end{pmatrix}
\begin{pmatrix}
A' \\
B \\
C \\
D'
\end{pmatrix}
= \begin{pmatrix}
0 \\
0 \\
0 \\
0
\end{pmatrix}
\]

Since the right-hand side is the zero vector, this set of equations will have only the trivial solution \( A' = B = C = D' = 0 \) (i.e. the wavefunction is uniformly zero) unless the determinant of the coefficient matrix is zero:

\[
\begin{vmatrix}
-1 & -\sin \xi & \cos \xi & 0 \\
0 & \sin \xi & \cos \xi & -1 \\
-\frac{\sqrt{K^2 - \xi^2}}{\xi} \cdot \cos \xi & \sin \xi & 0 \\
0 & \cos \xi & -\sin \xi & \sqrt{\frac{K^2 - \xi^2}{\xi}}
\end{vmatrix}
= 0
\]

or

\[
2\sqrt{\frac{K^2 - \xi^2}{\xi}} \left( \cos^2 \xi - \sin^2 \xi \right) + (\sin \xi \cos \xi) \left( 2 \frac{K^2}{\xi^2} - 4 \right) = 0
\]

upon a straightforward (if tedious) evaluation of the determinant. Using the double-angle formulas \( \cos 2\xi = \cos^2 \xi - \sin^2 \xi \) and \( \sin 2\xi = 2 \sin \xi \cos \xi \) and multiplying through by \( \xi^2 \), we get

\[
2\xi \sqrt{K^2 - \xi^2} \cos (2\xi) + (K^2 - 2\xi^2) \sin (2\xi) = 0
\]

which is the desired equation governing the energy spectrum (recall that \( \xi \) is a function of \( E \)).
As for the second form of the energy equation, it is probably easiest to see its equivalence to the first form by working backwards. That is, we start with the equation

$$\xi + \sin^{-1}\left(\frac{\xi}{K}\right) = \frac{n\pi}{2}$$

where \(n\) is some integer. Let us multiply both sides by 2 and then take the sine of both sides:

$$\sin\left[2\left(\xi + \sin^{-1}\left(\frac{\xi}{K}\right)\right)\right] = \sin n\pi$$

$$= 0 \quad \text{(because } n \text{ is integer)}$$

Then we expand the left-hand side using the sine angle-addition formula:

$$\sin (2\xi) \cos \left(2\sin^{-1}\left(\frac{\xi}{K}\right)\right) + \cos (2\xi) \sin \left(2\sin^{-1}\left(\frac{\xi}{K}\right)\right) = 0$$

Using the double-angle formulas only on the terms with inverse trig functions:

$$\sin (2\xi) \left\{ \cos^2 \left(\sin^{-1}\left(\frac{\xi}{K}\right)\right) - \sin^2 \left(\sin^{-1}\left(\frac{\xi}{K}\right)\right) \right\} + \cos (2\xi) \left\{ 2\sin \left(\sin^{-1}\left(\frac{\xi}{K}\right)\right) \cos \left(\sin^{-1}\left(\frac{\xi}{K}\right)\right) \right\} = 0$$

and with

$$\sin \left(\sin^{-1}\left(\frac{\xi}{K}\right)\right) = \frac{\xi}{K} \quad \text{and} \quad \cos \left(\sin^{-1}\left(\frac{\xi}{K}\right)\right) = \sqrt{1 - \left(\frac{\xi}{K}\right)^2} = \frac{\sqrt{K^2 - \xi^2}}{K}$$

we find

$$\sin (2\xi) \left\{ 1 - 2\frac{\xi^2}{K^2} \right\} + \cos (2\xi) \left\{ 2\frac{\xi}{K} \frac{\sqrt{K^2 - \xi^2}}{K} \right\} = 0$$

Multiplying through by \(K^2\), we recover the original form of the energy equation.

The final issue before us is how to calculate the wavefunction (i.e. the constants \(A, B, C, D\)) for a given value of the energy (as determined by some solution \(\xi\) of the energy equation). Since we set the determinant of the coefficient matrix to zero above, this means that our four equations above are not all independent: once we have considered three of the equations, the fourth equation becomes redundant, trivially satisfied as a consequence of the other three. (None of our four equations are special: we can pick any one of them to be the redundant one.) We are not going to worry about the overall normalization of the wavefunction, so we can follow the following simple procedure for a given \(\xi\): simply pick \(A' = 1\), and then given this choice, solve the first three of our four equations for \(B, C, D'\). As we have already stated, the values we find for \(A', B, C, D'\) will automatically satisfy the fourth equation.

This approach works perfectly well; however, in this problem we can be a little more clever. (Of course, it’s easy to be clever when we know the destination we are heading towards!) Let’s go back to our original four equations: the first two were

$$-B \sin \xi + C \cos \xi = A \exp \left(-\sqrt{K^2 - \xi^2}\right) = A'$$

$$B \sin \xi + C \cos \xi = D \exp \left(-\sqrt{K^2 - \xi^2}\right) = D'$$

If we solve for \(B, C\) in terms of \(A', D'\), we find

$$B = -\frac{A' - D'}{2 \sin \xi} \quad C = \frac{A' + D'}{2 \cos \xi}$$

We can do the same thing with the last two equations

$$B \cos \xi + C \sin \xi = \frac{\sqrt{K^2 - \xi^2}}{\xi} \cdot A'$$

$$B \cos \xi - C \sin \xi = -\frac{\sqrt{K^2 - \xi^2}}{\xi} \cdot D'$$
giving us

\[ B = \frac{\sqrt{K^2 - \xi^2}}{\xi} \cdot \frac{A' - D'}{2\cos \xi} \quad C = \frac{\sqrt{K^2 - \xi^2}}{\xi} \cdot \frac{A' + D'}{2\sin \xi} \]

If we demand that our two solutions for \( B \) be consistent, we find that

\[
\text{either } \tan \xi = -\frac{\xi}{\sqrt{K^2 - \xi^2}} \quad \text{or } A' = D', \quad B = 0.
\]

Meanwhile, consistency of the two solutions for \( C \) requires

\[
\text{either } \tan \xi = \frac{\sqrt{K^2 - \xi^2}}{\xi} \quad \text{or } A' = -D', \quad C = 0.
\]

Now it is easy to see that the conditions on \( \tan \xi \) cannot both be simultaneously true: setting them equal gives \( K^2 = 0 \) which is impossible. Likewise, they cannot both be false, or else the wavefunction becomes zero identically. We see that exactly one must be true and the other must be false. Therefore, our solutions fall into two classes:

- the first class satisfies \( \tan \xi = \frac{\sqrt{K^2 - \xi^2}}{\xi} \) and \( A' = D', B = 0 \). If we set \( A' = 1 \), we find \( D' = 1 \) and \( C = \frac{\sqrt{K^2 - \xi^2}}{\xi \sin \xi} \); so the complete (unnormalized) wavefunction is

\[
\psi_{\text{even}}(x) = \begin{cases} 
\exp \left( \frac{\sqrt{K^2 - \xi^2}}{\xi \cos \xi} \cdot \frac{L + x}{L} \right) & \text{for } x \leq -L \\
\frac{\sqrt{K^2 - \xi^2}}{\xi \cos \xi} \cdot \cos \left( \frac{\xi}{L} x \right) & \text{for } -L \leq x \leq L \\
-\exp \left( \frac{\sqrt{K^2 - \xi^2}}{\xi \cos \xi} \cdot \frac{L - x}{L} \right) & \text{for } x \geq L
\end{cases}
\]

We observe that these solutions have even parity! (i.e. they satisfy \( \psi(-x) = \psi(x) \)); hence the “even” label.

- the second class satisfies \( \tan \xi = -\frac{\xi}{\sqrt{K^2 - \xi^2}} \) and \( A' = -D', C = 0 \). If we set \( A' = 1 \), we find \( D' = -1 \) and \( B = \frac{\sqrt{K^2 - \xi^2}}{\xi \cos \xi} \), so the complete unnormalized wavefunction is

\[
\psi_{\text{odd}}(x) = \begin{cases} 
\exp \left( \frac{\sqrt{K^2 - \xi^2}}{\xi \cos \xi} \cdot \frac{L + x}{L} \right) & \text{for } x \leq -L \\
\frac{\sqrt{K^2 - \xi^2}}{\xi \cos \xi} \cdot \sin \left( \frac{\xi}{L} x \right) & \text{for } -L \leq x \leq L \\
-\exp \left( \frac{\sqrt{K^2 - \xi^2}}{\xi \cos \xi} \cdot \frac{L - x}{L} \right) & \text{for } x \geq L
\end{cases}
\]

These solutions have odd parity (they satisfy \( \psi(-x) = -\psi(x) \)).

The final thing that we should do is to go back to our energy equation, in the form

\[ \xi + \sin^{-1} \left( \frac{\xi}{K} \right) = \frac{n\pi}{2} \]

(where the integer \( n \) enumerates the energy states) and ask: for a given value of \( n \), which of the two classes does the solution fall into? To clear this up, we first write this equation as

\[ \xi = \frac{n\pi}{2} - \sin^{-1} \left( \frac{\xi}{K} \right) \]

from which it follows that

\[
\sin \xi = \sin \left( \frac{n\pi}{2} \right) \cos \left( \sin^{-1} \left( \frac{\xi}{K} \right) \right) - \cos \left( \frac{n\pi}{2} \right) \sin \left( \sin^{-1} \left( \frac{\xi}{K} \right) \right) = \sin \left( \frac{n\pi}{2} \right) \cdot \frac{\sqrt{K^2 - \xi^2}}{K} - \cos \left( \frac{n\pi}{2} \right) \cdot \frac{\xi}{K}
\]
and
\[
\cos \xi = \cos \left( \frac{n\pi}{2} \right) \cos \left( \sin^{-1} \left( \frac{\xi}{K} \right) \right) + \sin \left( \frac{n\pi}{2} \right) \sin \left( \sin^{-1} \left( \frac{\xi}{K} \right) \right)
\]

\[
= \cos \left( \frac{n\pi}{2} \right) \cdot \frac{\sqrt{K^2 - \xi^2}}{K} + \sin \left( \frac{n\pi}{2} \right) \cdot \frac{\xi}{K}
\]

so therefore

\[
\tan \xi = \frac{\sin \xi}{\cos \xi} = \frac{\sin \left( \frac{n\pi}{2} \right) \cdot \frac{\sqrt{K^2 - \xi^2}}{K} - \cos \left( \frac{n\pi}{2} \right) \cdot \frac{\xi}{K}}{\cos \left( \frac{n\pi}{2} \right) \cdot \frac{\sqrt{K^2 - \xi^2}}{K} + \sin \left( \frac{n\pi}{2} \right) \cdot \frac{\xi}{K}}
\]

We now consider two cases:

- If \( n \) is odd, then \( \cos \left( \frac{n\pi}{2} \right) = 0 \), and so \( \tan \xi = \frac{\sqrt{K^2 - \xi^2}}{\xi} \). This is the condition for the first class of solutions, which have even parity.

- If \( n \) is even, then \( \sin \left( \frac{n\pi}{2} \right) = 0 \), and so \( \tan \xi = -\frac{\xi}{\sqrt{K^2 - \xi^2}} \). These solutions fall into the second class, and have odd parity.

So at last we have completely characterized the energy eigenvalues and eigenfunctions.

note: We could have noticed right at the beginning that the Hamiltonian was invariant under parity, and so the (nondegenerate) eigenfunctions were required to have a definite parity. Thus instead of writing down the most general solution to Schrödinger’s equation as we did above, we could have written down even-and odd-parity solutions, and found the energy equation for each case. I won’t go through the details (the problem is solved in this manner in Griffiths, for example), but notice that this approach gives you two energy equations (one for each parity). These equations, in our notation and our setup, are

\[
\xi \tan \xi = \sqrt{K^2 - \xi^2} \quad \text{and} \quad \xi \cot \xi = -\sqrt{K^2 - \xi^2}
\]

(if you compare with Griffiths, keep in mind that all his energies are shifted by \( V_0 \) with respect to ours!)

To get the one energy equation as given in this problem, we simply write down one equation which has the above two equations as roots:

\[
\left( \xi \tan \xi - \sqrt{K^2 - \xi^2} \right) \left( \xi \cot \xi + \sqrt{K^2 - \xi^2} \right) = 0
\]

Now just multiply out the left-hand side, and use the double-angle formulas (after writing tan & cot in terms of sin & cos). The result is our energy equation.

(b) As in the previous problem, sketch the wave function for the ground state and the two excited states (i.e. for \( n=1,2,3 \)) and point out the key differences between these single particle states and those in an \textit{infinite} potential well.

We can notice one very important difference just by inspecting the energy equation

\[
\xi + \sin^{-1} \left( \frac{\xi}{K} \right) = \frac{n\pi}{2}
\]

where \( \xi = L\sqrt{2mE}/\hbar^2 \), \( K = L\sqrt{2mV_0}/\hbar^2 \), and \( n \) is an integer.

The argument of \( \sin^{-1} \) must be less than or equal to one, so the left-hand side is defined only for \( 0 \leq \xi \leq K \).

(It would also be defined for negative \( \xi \), but the definition of \( \xi \) prevents this from happening.) But the left-hand side is a monotonically increasing function of \( \xi \), so its value must be between \( 0 \) and \( K + \sin^{-1} 1 = K + \pi/2 \).

That is, the left-hand side has a maximum; if \( n \) becomes too large then this equation will not have a solution.

In fact, the only values of \( n \) which work are those for which

\[
\frac{n\pi}{2} \leq K + \frac{\pi}{2}
\]
So whereas there were an infinite number of bound states in the infinite square well, the number of states in the finite potential well is

\[ 1 + \left\lfloor \frac{2}{\pi K} \right\rfloor \]

where \( [x] \) means that we round down \( x \) to the nearest integer. (Notice, by the way, that the well will always have at least one bound state, no matter how shallow it is; this state will have even parity, since it has \( n = 1 \).)

For this problem, we want there to be at least three bound states, so we need to choose a value of \( K \) which allows this. The condition on \( K \) will be \( K \geq \pi \); let us choose \( K = 4 \) for definiteness. Then we can use numerical methods to find \( \xi \) for \( n = 1, 2, 3 \); the result is

\[ \xi_1 = 1.25235, \quad \xi_2 = 2.47458, \quad \xi_3 = 3.59530 \]

We take these values and plug them into the expressions found in part (a), using \( \psi_{\text{even}} \) for the even-parity states \( n = 1, 3 \) and \( \psi_{\text{odd}} \) for the odd-parity \( n = 2 \). The results for the wavefunctions and the corresponding probability densities are shown below: (the vertical lines show the edges of the well)

![Wavefunction plots](image)

(note: these are the normalized wavefunctions! Normalization causes \( \psi \) to be multiplied by some constant; it is possible to show, after some tedious computation and judicious use of the energy quantization conditions, that the normalization factor for both even-parity and odd-parity solutions is

\[ N = \frac{1}{\sqrt{L K}} \sqrt{\frac{\sqrt{K^2 - \xi^2}}{1 + \sqrt{K^2 - \xi^2}}} \]

i.e. the normalized wavefunctions are \( N \psi_{\text{even/odd}} \).)

We note some similarities with the case of the infinite potential well: the \( n^{\text{th}} \) energy state possesses \( n - 1 \) nodes inside the well, and states with odd (even) \( n \) have even (odd) parity with respect to the center of the well. There are also a few key differences: of course, the wavefunction is no longer zero outside the well. Also, the edges of the well are no longer nodes.

One other thing we see from the graph of \(|\psi|^2\) is that states with higher \( n \) are more likely to be found outside the well. This makes sense because these states have higher energy, and so are less inclined to be confined within the well. (Notice, by the way, that we needed to normalize our wavefunctions, in order to be able to compare different wavefunctions on the graph.)

(c) Discuss the behavior of the wave function in the classically forbidden region and extract the so called “characteristic tunneling length”. Estimate the tunneling length for an electron with energy 25 eV in a well with \( L = 1\text{A} \) and \( V_0 = 100 \text{ eV} \).

What we have found is that in the classically forbidden regime, where the potential exceeds the particle’s energy, the wavefunction takes the form of a decaying exponential. The tunneling length is the way in which
we characterize how fast the exponential is dying off; a simply way to define it is the length scale in which the wavefunction decreases by a factor of \( e \) from its maximum value. This corresponds to the argument of our exponentials decreasing from 0 to -1. Let’s look, for instance, at \( \psi_{\text{even}} \) for \( x \geq L \) (other cases will give the same result). The wave function is proportional to

\[
\exp \left( \sqrt{K^2 - \xi^2} \cdot \frac{L - x}{L} \right);
\]

the argument of the exponential is zero at \( x = L \) and goes to -1 at \( x = L \left( 1 + \frac{1}{\sqrt{K^2 - \xi^2}} \right) \). Therefore, the tunneling length equals the change in \( x \), or just

\[
\frac{L}{\sqrt{K^2 - \xi^2}} = \frac{L}{\sqrt{2m(V_0 - E)L^2}} = \frac{\hbar c}{\sqrt{2mE}(V_0 - E)}
\]

Notice that the tunneling length does not depend on \( L \); tunneling occurs outside the well and is not affected by \( L \) which measures the region inside the well (the classically allowed region).

With \( V_0 - E = 75 \text{ eV}, \ mc^2 \approx 511 \times 10^3 \text{ eV} \) for an electron, and \( \hbar c \approx 197 \text{ eV} \cdot \text{nm} \), the tunneling length evaluates to 0.23 \( \text{Å} \).

3. Let us now look at scattering off a tunnel barrier described by the following potential profile: \( V(x) = V_0 \) for \( 0 \leq x \leq L \) and \( V(x) = 0 \) otherwise. \( \text{[i.e. we have } 0 < E < V_0 \text{ where } E \text{ is the particle energy].} \)

(a) Show that the amplitude \( D \) of the transmitted wave is (for simplicity, let us normalize the amplitude of the incident wave to unity \( A_0 = 1 \))

\[
D = \frac{4ik_1k_2e^{-ik_1L}}{(k_2 + ik_1)^2 e^{-k_2L} - (k_2 - ik_1)^2 e^{+k_2L}}
\]

where \( k_1 \equiv \sqrt{2mE}/\hbar \) and \( k_2 = \sqrt{2m(V_0 - E)}/\hbar \).

In the regions outside the barrier, where \( V = 0 \) and so \( E > V \), the solutions will be plane waves characterized by \( k_1 \); inside the barrier, where \( E < V \), the solutions will be exponentially characterized by \( k_2 \). We then write down the general form of the wavefunction:

\[
\psi(x) = \begin{cases} 
  e^{ik_1x} + Ae^{-ik_1x}, & x \leq 0 \\
  Be^{k_2x} + Ce^{-k_2x}, & 0 \leq x \leq L \\
  De^{ik_1x}, & x \geq L
\end{cases}
\]

For \( x \leq 0 \), we have an incident wave with amplitude 1 as suggested (this will not cause any difficulties, since we will be concerned in this problem with the \( \text{sums of various amplitudes} \) and a reflected wave; inside the barrier we have our two exponentials; and for \( x \geq L \) we have just a transmitted wave (the other exponential is not present, since no reflection at \( x = +\infty \) takes place.

The values of the constants \( A, B, C, D \) are fixed by enforcing continuity of \( \psi \) and \( \psi' \) at the boundaries between regions:

\[
\begin{align*}
\psi(0^-) &= \psi(0^+) \quad \Rightarrow \quad 1 + A = B + C \\
\psi'(0^-) &= \psi'(0^+) \quad \Rightarrow \quad ik_1(1 - A) = k_2(B - C) \\
\psi(L^-) &= \psi(L^+) \quad \Rightarrow \quad Be^{k_2L} + Ce^{-k_2L} = De^{ik_1L} \\
\psi'(L^-) &= \psi'(L^+) \quad \Rightarrow \quad k_2(Be^{k_2L} - Ce^{-k_2L}) = ik_1De^{ik_1L}
\end{align*}
\]
We solve the third & fourth equations for $B, C$ in terms of $D$:

$$B = \frac{1}{2} e^{-k_2 L} \left( 1 + \frac{ik_1}{k_2} \right) D e^{ik_1 L} = (k_2 + ik_1) e^{-k_2 L} \cdot \frac{D e^{ik_1 L}}{2k_2}$$

$$C = \frac{1}{2} e^{k_2 L} \left( 1 - \frac{ik_1}{k_2} \right) D e^{ik_1 L} = (k_2 - ik_1) e^{k_2 L} \cdot \frac{D e^{ik_1 L}}{2k_2}$$

Next we combine the first and second equations by eliminating $A$:

$$2 = B + C \frac{k_2}{ik_1} (B - C)$$

or

$$2ik_1 = B (k_2 + ik_1) - C (k_2 - ik_1)$$

Now substitute in for $B$ and $C$:

$$2ik_1 = \frac{D e^{ik_1 L}}{2k_2} \left\{ (k_2 + ik_1)^2 e^{-k_2 L} - (k_2 - ik_1)^2 e^{k_2 L} \right\}$$

Solving for $D$ yields the desired result.

(b) Use the above result to compute the so-called transmission coefficient $T \equiv DD^*$ and show that

$$T = \frac{1}{1 + \left( \frac{k_2^2 + k_3^2}{2ik_1k_2} \right)^2 \sinh^2 (k_2 L)}$$

Let us consider a generic plane wave $a \cdot e^{ikx}$ travelling in the positive $x$-direction. Let us calculate the probability flux $j_x$ associated with this wave function: in one dimension, we have

$$j_x = \frac{\hbar}{2mi} \left( \psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right)$$

$$= \frac{\hbar}{2mi} a^* a \left( (e^{-ikx}) (ie^{ikx}) - (e^{ikx}) (i e^{-ikx}) \right)$$

$$= \frac{\hbar k}{m} |a|^2$$

For a wave travelling in the opposite direction $a \cdot e^{-ikx}$, we find $j_x = -\frac{\hbar k}{m} |a|^2$. We see that for each wave, we have a steady flow of probability density in the same direction as the wave; that is, each wave describes a steady flow of particles in a given direction.

Now, in our scattering setup, the incident wave acts as a continuous source of particles, some of which end up in the transmitted wave and some in the reflected wave. It is then natural to generically define the transmission coefficient as the fraction of the incoming probability flux which gets transmitted: in one dimension,

$$T = \frac{j_{x, \text{trans}}}{j_{x, \text{incident}}}$$

Our incident wave has the form $1 \cdot e^{ik_1 x}$, while the transmitted wave is $D \cdot e^{ik_1 x}$; so we have

$$T = \frac{\frac{\hbar k}{m} |D|^2}{\frac{\hbar k}{m} 1} = |D|^2 = DD^*$$

This justifies the definition given in the problem. For the value of $D$ found in part (a), we have (remembering that $k_1$ and $k_2$ are purely real)

$$DD^* = \frac{4ik_1k_2 e^{-ik_1 L}}{(k_2 + ik_1)^2 e^{-k_2 L} - (k_2 - ik_1)^2 e^{k_2 L}} \left( \frac{4ik_1k_2 e^{ik_1 L}}{(k_2 - ik_1)^2 e^{-k_2 L} - (k_2 + ik_1)^2 e^{k_2 L}} \right)$$

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\[
\frac{16k_1^2 k_2^2}{(k_2^2 + k_1^2)^2 (e^{-2k_2L} + e^{2k_2L}) - (k_2 + ik_1)^4 - (k_2 - ik_1)^4}
\]
\[
 = \frac{16k_1^2 k_2^2}{(k_2^2 + k_1^2)^2 (e^{-2k_2L} + e^{2k_2L}) - 2k_1^4 - 2k_2^4 + 12k_1^2 k_2^2}
\]
\[
 = \frac{16k_1^2 k_2^2}{(k_2^2 + k_1^2)^2 (e^{-2k_2L} + e^{2k_2L} - 2) + 16k_1^2 k_2^2}
\]
\[
 = \frac{1}{(k_2^2 + k_1^2)^2 (e^{k_2L} - e^{-k_2L})^2 + 16k_1^2 k_2^2}
\]
\[
 = \frac{1}{1 + \left(\frac{k_2^2 + k_1^2}{2k_1 k_2}\right)^2 \sinh^2 (k_2L)}
\]

(c) Derive the limiting forms of \( T \) for the so-called thick barrier \((k_2L > 1)\) and thin barrier \((k_2L \ll 1)\) cases, and show that

\[
T_{\text{thick}} = 16 \left( \frac{E}{V_0} \right) \left( 1 - \frac{E}{V_0} \right) \exp \left[ -\frac{2L}{\hbar} \sqrt{2m(V_0 - E)} \right]
\]
\[
T_{\text{thin}} = 1 - \frac{mV_0^2 L^2}{2E \hbar^2}
\]

[please note the corrections to the definitions of thick & thin barrier, and to the formula for \( T_{\text{thin}}, as compared to the question sheets which were distributed to students/]

Consider first the thick barrier. When \( x \gg 1 \), we have \( e^x \gg 1 \) and \( e^{-x} \ll 1 \), and so

\[
\sinh x \equiv \frac{e^x - e^{-x}}{2} \approx \frac{e^x}{2}
\]

Moreover, from the final form of the approximation, we will have also \( \sinh x \gg 1 \). So in the formula for \( T \), we can make the approximation for \( \sinh \) shown here, and we can also neglect the 1 in the denominator compared to the \( \sinh \) term:

\[
T_{\text{thick}} \approx \frac{1}{(k_1^2 + k_2^2)^2 \left( \frac{e^{k_2L}}{2} \right)^2}
\]
\[
= \left( \frac{4k_1 k_2}{k_1^2 + k_2^2} \right)^2 e^{-2k_2L}
\]
\[
= \frac{16 k_1^2 k_2^2}{(k_1^2 + k_2^2)^2} e^{-2k_2L}
\]

Using \( k_1^2 = \frac{2mE}{\hbar^2} \) and \( k_2^2 = \frac{2m(V_0 - E)}{\hbar^2} \), we have

\[
T_{\text{thick}} = 16 \left( \frac{2mE}{\hbar^2} \right)^2 \frac{E(V_0 - E)}{(2mV_0)^2} \exp \left[ -2L \cdot \frac{2m(V_0 - E)}{\hbar^2} \right]
\]
\[
= 16 \left( \frac{E}{V_0} \right) \left( 1 - \frac{E}{V_0} \right) \exp \left[ -\frac{2L}{\hbar} \sqrt{2m(V_0 - E)} \right]
\]

as desired.
For the thin barrier, we use the approximation for \( x \ll 1 \) that
\[
\sinh x = \frac{e^x - e^{-x}}{2} \approx \frac{(1 + x) - (1 - x)}{2} = x
\]
to write
\[
T_{\text{thin}} \approx \frac{1}{1 + \left( \frac{k_1^2 + k_2^2}{2k_1k_2} \right)^2 (k_2 L)^2}
\]
Then, still keeping in mind that \( k_2 L \ll 1 \), we can use the further approximation \((1 + x)^{-1} \approx 1 - x\):
\[
T_{\text{thin}} \approx 1 - \left( \frac{k_1^2 + k_2^2}{2k_1k_2} \right)^2 (k_2 L)^2
\]
\[
= 1 - \frac{L^2}{4k_1^2} (k_1^2 + k_2^2)^2
\]
\[
= 1 - \frac{L^2}{4} \left( \frac{2mV_0}{\hbar^2} \right)^2
\]
\[
= 1 - \frac{mV_0^2 L^2}{2E\hbar^2}.
\]

(d) Argue that alpha-decay can be viewed as a barrier penetration effect.

The alpha decay of a nucleus involves 2 protons and 2 neutrons (i.e. a nucleus of helium) detaching from the nucleus and escaping as a unit. Observed kinetic energies of the alpha particle are on the order of MeV. Now, the protons within a nucleus, being positively charged, repel each other via Coulomb forces. What holds the nucleus together is the strong force: an attraction between nucleons which dominates the Coulomb repulsion, but which acts with a very short range. In fact, we can think of this force as acting only within the nucleus itself. Then, consider an alpha particle attempting to leave a nucleus of size \( R \); it can essentially move freely within the nucleus, but when it attempts to leave, it suddenly experiences only the repulsive Coulomb potential. The problem is that the magnitude of the Coulomb potential at the “surface” of a nucleus typically greatly exceeds the kinetic energy of the alpha particles that we see! Indeed, for a moderate-Z nucleus \( (Z \approx 60) \) with a typical nuclear size of 5 fm, the electrostatic potential energy between the alpha particle and the nucleus equals

\[
\frac{1}{4\pi\varepsilon_0} \frac{(2e)(60e)}{5 \text{ fm}} \approx 35 \text{ MeV}
\]
which is an order of magnitude larger than the typical alpha particle kinetic energy. So, the Coulomb potential should act as an energy barrier which the alpha is unable to cross.

Then how does the alpha particle leave? Simple – it tunnels across the energy barrier! Using a tunneling model, it is possible to write down accurate quantitative relationships between the alpha kinetic energy and the decay rate (i.e. the probability of tunneling).

4. This problem is devoted to scattering by a 1-D potential well: \( V(x) = -V_0 \) for \( 0 \leq x \leq L \) and \( V(x) = 0 \) otherwise. \([\text{Here } E > 0 \text{ and } V_0 > 0].\)

(a) Show that the transmission coefficient (defined the same way as in the previous problem) is given by
\[
T = \frac{4k_1^2 k_2^2}{(k_1^2 + k_2^2)^2 - (k_2^2 - k_1^2)^2 \cos^2 (k_2 L)}
\]

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where \( k_1 = \sqrt{2mE/\hbar} \) and \( k_2 = \sqrt{2m(E + V_0)/\hbar} \).

The method of solution is essentially the same as in the previous problem, the principal difference being that the wavefunction inside the well consists of plane waves rather than exponentials, since the energy exceeds the potential in the well. Without further ado, we write down the general form of the wavefunction:

\[
\psi(x) = \begin{cases} 
  e^{ik_1x} + A e^{-ik_1x}, & x \leq 0 \\
  Be^{ik_2x} + C e^{-ik_2x}, & 0 \leq x \leq L \\
  D e^{ik_1x}, & x \geq L 
\end{cases}
\]

where \( k_1 \) and \( k_2 \) are defined in the problem (and note that \( k_2 \) in this problem is different from the \( k_2 \) in problem \#3).

Again we enforce continuity of \( \psi \) and \( \psi' \) on the boundaries:

\[
\begin{align*}
\psi^-(0^-) &= \psi^+(0^+) &\Rightarrow 1 + A = B + C \\
\psi'^-(0^-) &= \psi'^+(0^+) &\Rightarrow ik_1 (1 - A) = ik_2 (B - C) \\
\psi^-(L^-) &= \psi^+(L^+) &\Rightarrow Be^{ik_2L} + C e^{-ik_2L} = De^{ik_1L} \\
\psi'^-(L^-) &= \psi'^+(L^+) &\Rightarrow ik_2 (Be^{ik_2L} - C e^{-ik_2L}) = ik_1 De^{ik_1L}
\end{align*}
\]

To get the transmission coefficient, we first need the transmitted wave amplitude \( D \). Now we can save ourselves a lot of algebra, by noticing that these equations are exactly the same as in problem 3a, except that \( k_2 \) has been replaced by \( ik_2 \) everywhere. So, we can take our solution for \( D \) from that problem and simply make the substitution \( k_2 \to ik_2 \), to get \( D \) for this problem:

\[
D = \frac{4ik_1 (ik_2) e^{-ik_1L}}{((ik_2) + ik_1)^2 e^{-(ik_2)L} - ((ik_2) - ik_1)^2 e^{+(ik_2)L}}
\]

or, dividing top and bottom by \( i^2 \):

\[
D = \frac{4k_1 k_2 e^{-ik_1L}}{(k_2 + k_1)^2 e^{-(ik_2)L} - (k_2 - k_1)^2 e^{+(ik_2)L}}
\]

Now we calculate the transmission coefficient \( T = |D|^2 \). Since we have taken the trouble of writing the denominator of \( D \) explicitly as real part plus imaginary part, taking the magnitude becomes very easy:

\[
T = \frac{(2k_1 k_2)^2 \cdot 1}{((k_2 + k_1)^2 \sin (k_2L))^2 + (2k_1 k_2 \cos (k_2L))^2}
\]

\[
= \frac{1}{(k_2 + k_1)^2 + \cos^2 (k_2L) \left\{ (2k_1 k_2)^2 - (k_2^2 + k_1^2)^2 \right\}}
\]

\[
= \frac{4k_1^2 k_2^2}{(k_2 + k_1)^2 + \cos^2 (k_2L) (2k_1 k_2 + k_2^2 + k_1^2) (2k_1 k_2 - k_2^2 - k_1^2)}
\]

\[
= \frac{4k_1^2 k_2^2}{(k_2 + k_1)^2 - \cos^2 (k_2L) (k_2 + k_1)^2 (k_2 - k_1)^2}
\]

\[
= \frac{4k_1^2 k_2^2}{(k_2 + k_1)^2 - (k_2 - k_1)^2 \cos^2 (k_2L)}
\]
as desired.

(b) Show that in the low-energy scattering limit $E \ll V_0$ the transmission coefficient $T(E) \propto E \frac{E}{V_0}$, since $T$ is dimensionless.

First let us write rewrite $T$ in terms of $V_0$ and $E$ rather than $k_1$ and $k_2$ (mostly), using $k_1^2 = \frac{2mE}{h^2}$ and $k_2^2 = \frac{2m(E + V_0)}{h^2}$:

$$T = \frac{4 \cdot \left(\frac{2m}{h^2}\right)^2 E (E + V_0)}{(2m)^2 (2E + V_0)^2 - \left(\frac{2m}{h^2}\right)^2 V_0^2 \cos^2 (k_2 L)}$$

$$= \frac{4E (E + V_0)}{(2E + V_0)^2 - V_0^2 \cos^2 (k_2 L)}$$

Now take the limit $E \ll V_0$. The easiest way to do this is to rewrite the desired limit as $\frac{E}{V_0} \ll 1$: i.e. $\frac{E}{V_0}$ is a small parameter. To make this parameter “appear” in our expression for $T$, we divide the top and bottom by $V_0^2$:

$$T = \left(\frac{4 \frac{E}{V_0} \left(\frac{E}{V_0} + 1\right)}{(2 \frac{E}{V_0} + 1)^2 - \cos^2 (k_2 L)}\right) \approx \frac{4 \frac{E}{V_0} \cdot 1}{1 - \cos^2 (k_2 L)}$$

In this problem, we need only the leading order approximation: that is, we simply neglect the small parameter compared to 1:

$$T \approx \frac{4 \frac{E}{V_0} \cdot 1}{1 - \cos^2 (k_2 L)} = \frac{E}{V_0} \cdot 4 \csc^2 (k_2 L)$$

So we have obtained the desired form. (We have not been careful about factors of $\frac{E}{V_0}$ arising from the $k_2$ present in the argument of the trig function: remember that $k_2 \equiv \sqrt{2m(E + V_0)/h} = \sqrt{2mV_0 \left(1 + \frac{E}{V_0}\right)/h}$. However, since we are only concerned with leading order, we just take $k_2 \approx \sqrt{2mV_0}/h$.)

(c) Show that in the high-energy scattering limit $E \gg V_0$ the transmission coefficient $T(E) \propto 1$.

Now our small parameter is $\frac{V_0}{E} \ll 1$. To make this parameter appear, we divide top and bottom by $4E^2$:

$$T = \frac{1 + \frac{V_0}{E}}{(1 + \frac{1}{2} \frac{V_0}{E})^2 - \frac{1}{4} \left(\frac{V_0}{E}\right)^2 \cos^2 (k_2 L)}$$

$$= \frac{1 + \frac{V_0}{E}}{1 + \frac{V_0}{E} + \frac{1}{4} \left(\frac{V_0}{E}\right)^2 \sin^2 (k_2 L)}$$

Again we are interested only in the leading order: we neglect the small parameter compared to 1, with the result $T \approx 1$.

(d) Find the so-called resonance conditions, i.e. the energies for which the structure becomes transparent and perfect transmission $T = 1$ is possible.

Let’s look at the last form for $T$ that we found in part (c) (i.e. the equation immediately preceding this part). We see immediately that the condition for $T$ to be 1 is

$$\frac{1}{4} \left(\frac{V_0}{E}\right)^2 \sin^2 (k_2 L) = 0$$
which is satisfied if
\[ k_2 L = n\pi \quad (n \text{ integer}) \]
or, substituting in for \( k_2 \) and solving for the energy:
\[ E = \frac{n^2 \pi^2 \hbar^2}{2mL^2} - V_0 \]
(\text{where } n \text{ must be sufficiently large that } E > 0, \text{ since we are talking about a scattering problem.})

We can understand our result by solving for \( L \) in the previous equation,
\[ L = \frac{n\pi}{k_2} = \frac{n}{2} \cdot \frac{2\pi}{k_2} \]
and recognizing \( \frac{2\pi}{k_2} \) as the de Broglie wavelength of the particle inside the well; so our condition says that the thickness of the well must be a multiple of half-multiple of the particle’s de Broglie wavelength for perfect transmission. But this makes perfect sense—imagine an incident wave encountering the well. Then the total reflected wave is the superposition of reflections from the front edge of the well (at \( x = 0 \)) and from the back edge (at \( x = L \)); moreover, reflections from the back edge include a 180° phase shift (entirely analogous to the situation in optics, where a light ray acquires such a phase shift when reflected at a boundary leading to a higher index of refraction). So these two sources of reflections will interfere destructively, and there will be no net reflected wave!

5. Read the paper by Don Eigler and his collaborators (M.F. Crommie, C.P. Lutz, and D.M. Eigler, Science 262, 218 (1993)). Follow the authors’ suggestion and model the corral of 48 iron atoms as a continuous hard-wall barrier which provides a round 2D “box” for a surface electron.

(a) Write down the Schrödinger equation for this problem exhibiting cylindrical symmetry, and show that the eigenfunctions are Bessel functions of the form mentioned in the article: \( \Psi_{n,l}(r, \phi) \propto J_l(k_{n,l}r) e^{i\phi} \). Here, \( l \) is the angular momentum of the electron, \( J_l \) is the \( l \)-th order Bessel function [of the first kind], and \( z_{n,l} \) is the \( n \)-th zeros crossing of \( J_l \). [And, \( k_{n,l} = z_{n,l}/R \), where \( R \) is the radius of the box.]

Inside the box, the electron acts like a free particle, and so its behavior is governed by a 2D free-particle Schrödinger equation:

\[-\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \psi(x, y) = E \psi(x, y)\]

We obviously would like to work in polar coordinates, so we need to rewrite the 2D Laplacian in polar coordinates. For reference, we write out the coordinate transformation:
\[
\begin{align*}
  x &= r \cos \phi & \rho &= \sqrt{x^2 + y^2} \\
  y &= r \sin \phi & \phi &= \tan^{-1} \left( \frac{y}{x} \right)
\end{align*}
\]

We calculate the needed partial derivatives:
\[
\begin{align*}
  \frac{\partial \rho}{\partial x} &= \frac{2x}{2\sqrt{x^2 + y^2}} = \cos \phi \\
  \frac{\partial \rho}{\partial y} &= \frac{2y}{2\sqrt{x^2 + y^2}} = \sin \phi \\
  \frac{\partial \phi}{\partial x} &= \frac{-y}{1 + \left( \frac{y}{x} \right)^2} = \frac{-y}{x^2 + y^2} = -\frac{\sin \phi}{\rho} \\
  \frac{\partial \phi}{\partial y} &= \frac{1}{1 + \left( \frac{y}{x} \right)^2} = \frac{x}{x^2 + y^2} = \frac{\cos \phi}{\rho}
\end{align*}
\]
Then
\[
\frac{\partial}{\partial x} = \frac{\partial_p}{\partial x} \frac{\partial}{\partial p} + \frac{\partial}{\partial x} \frac{\partial}{\partial \phi} = (\cos \phi) \frac{\partial}{\partial p} - \left( \frac{\sin \phi}{\rho} \right) \frac{\partial}{\partial \phi},
\]
and
\[
\frac{\partial}{\partial y} = \frac{\partial_p}{\partial y} \frac{\partial}{\partial p} + \frac{\partial}{\partial y} \frac{\partial}{\partial \phi} = (\sin \phi) \frac{\partial}{\partial p} + \left( \cos \phi \right) \frac{\partial}{\partial \phi},
\]
so
\[
\frac{\partial^2 f}{\partial x^2} = (\cos \phi) \frac{\partial}{\partial p} \left( \frac{\sin \phi}{\rho} \frac{\partial}{\partial \phi} \right) \left( \frac{\partial}{\partial p} \frac{\partial f}{\partial p} - \frac{\sin \phi}{\rho} \frac{\partial f}{\partial \phi} \right)
= \left( \cos^2 \phi \right) \frac{\partial^2 f}{\partial p^2} - \left( \frac{\sin \phi}{\rho} \right) \frac{\partial f}{\partial p \partial \phi} + \frac{\sin^2 \phi}{\rho^2} \frac{\partial^2 f}{\partial \phi^2}
\]
and
\[
\frac{\partial^2 f}{\partial y^2} = \left( \frac{\sin \phi}{\rho} \right) \frac{\partial \phi}{\partial f} \left( \frac{\cos \phi}{\rho} \frac{\partial}{\partial \phi} + \frac{\cos \phi}{\rho} \frac{\partial}{\partial \phi} \right) \left( \frac{\partial}{\partial p} \frac{\partial f}{\partial p} + \frac{\cos \phi}{\rho} \frac{\partial f}{\partial \phi} \right)
= \left( \sin^2 \phi \right) \frac{\partial^2 f}{\partial p^2} + \left( \frac{\sin \phi}{\rho} \right) \frac{\partial f}{\partial p \partial \phi} - \frac{\sin^2 \phi}{\rho^2} \frac{\partial^2 f}{\partial \phi^2}
\]
Adding these results, we have finally
\[
\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = \frac{1}{\rho} \frac{\partial f}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2 f}{\partial \phi^2}
\]
so the Schrödinger equation becomes
\[
-\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} \right) \psi (\rho, \phi) = E \psi (\rho, \phi)
\]
(This is obviously not the most efficient way to derive the form of the Laplacian in polar coordinates, but it is the most elementary.)

As is typically done, we solve this partial differential equation by separation of variables: we substitute in a separated solution, of the form
\[
\psi (\rho, \phi) \equiv P (\rho) \Phi (\phi)
\]
with the result
\[
\Phi \cdot \left( \frac{d^2 P}{d\rho^2} + \frac{1}{\rho} \frac{dP}{d\rho} + \frac{P}{\rho^2} \frac{d^2 \Phi}{d\phi^2} \right) = \frac{2mE}{\hbar^2} P \Phi
\]
Then we divide through by \( \psi = P \Phi \), and isolate the \( \phi \)-dependent stuff on one side of the equation:
\[
\frac{1}{P} \left( \frac{d^2 P}{d\rho^2} + \frac{1}{\rho} \frac{dP}{d\rho} + \frac{P}{\rho^2} \frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} \right) = -\frac{2mE}{\hbar^2}
\]
or,
\[
\frac{\rho^2}{P} \left( \frac{d^2 P}{d\rho^2} + \frac{1}{\rho} \frac{dP}{d\rho} + \frac{2mE}{\hbar^2} \rho^2 \right) = -\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2}
\]
The left-hand side is a function of $\rho$ alone, the right-hand side only of $\phi$; as they are equal, they must both equal some constant which is independent of both variables. We call this constant $l^2$; then we have two ordinary differential equations:

$$\frac{d^2 P}{d\rho^2} + \frac{1}{\rho} \frac{dP}{d\rho} + \left( \frac{2mE}{\hbar^2} - \frac{l^2}{\rho^2} \right) P = 0$$

and

$$\frac{d^2 \Phi}{d\phi^2} + l^2 \Phi = 0$$

There is no a priori restriction on the value of the constant $l^2$; despite our notation for the constant, it could in principle be negative. However, we require that the wavefunction be single-valued at any physical point, which imposes the condition that $\Phi (\phi + 2\pi) = \Phi (\phi)$ for any $\phi$. Now, for positive $l^2$, the solutions of the $\Phi$ differential equation are linear combinations of $e^{il\phi}$ and $e^{-il\phi}$, so single-valuedness requires that $l$ be an integer. For negative $l^2$, the solutions are combinations of $e^{il\phi}$ and $e^{-il\phi}$, and it is easy to show that the single-valuedness for all $\phi$ is impossible; so this case is ruled out.

We now define $k^2 = 2mE/\hbar^2$, and look at the $P$ differential equation,

$$\frac{d^2 P}{d\rho^2} + \frac{1}{\rho} \frac{dP}{d\rho} + \left( k^2 - \frac{l^2}{\rho^2} \right) P = 0$$

where, as we found, $l$ is an integer. This is a standard differential equation of mathematical physics, known as Bessel's equation. Its solutions are linear combinations of Bessel functions of the first and second kind, specifically $J_l(k\rho)$ and $Y_l(k\rho)$. (A basic introduction to the properties of Bessel functions can be found in Jackson, Classical Electrodynamics, 3rd ed, chapter 3, or in Arfken & Weber, Mathematical Methods for Physicists, 5th ed, chapter 11.) One property of these functions is that as $x \to 0$, $J_l(x)$ stays finite while $Y_l(x)$ diverges; with the reasonable requirement that the wavefunction be finite everywhere, we can rule out the $Y_l$ solutions entirely.

Finally, we use the fact that the electron is confined in a 2D box of radius $R$ to give us a final boundary condition: since $\Psi$ is zero outside the box, and $\Psi$ is continuous, we require that $P(\rho) |_{\rho=R} = 0$, i.e.

$$J_l(kR) = 0$$

For each integer $l$, the Bessel function $J_l$ has an infinite set of zeroes, whose values are denoted as $z_{n,l}$ ($n = 1, 2, 3, \ldots$); so our condition can be rewritten as

$$k_{n,l} = \frac{z_{n,l}}{R} \Rightarrow E_{n,l} = \frac{\hbar^2 z_{n,l}^2}{2mR^2}$$

where we have added the $n, l$ subscripts to $k$ and $E$ to remind us that the allowed energies are now quantized, as a consequence of the electron being confined in a box.

So we have established that the eigenfunctions take the form $J_l(k_{n,l}\rho) e^{il\phi}$.

(b) See if you can reproduce qualitatively the local density of states, LDOS $\propto |\Psi(\rho, \phi)|^2$, seen in the scanning tunneling (STM) microscopy experiment. You may want to try a single eigenstate first, but note that the authors used a linear combination of several states to quantitatively fit the data (see the caption for fig. 2 in the paper).

Without going into the details of the experiment, we effectively have many electrons confined in our box, which fill up the energy states from the lowest energy on upwards. The energy of the highest filled state is known as the Fermi energy $E_F$; the STM technique probes the probability density of electrons in this highest filled state, which will be proportional to $J^2_l(k_{n,l}\rho)$ for some $n, l$. For the particular measurement described in the paper, it happened that there were other states with energies very near to $E_F$; when the energies are sufficiently close, STM will probe $|\Psi|^2$ for these states as well with roughly equal weight.

The states in question have $(n, l) = (5, 0), (4, 2), (2, 7)$. To plot the probability densities, we need to know the values of the corresponding Bessel-function zeroes: i.e. we need the 5th zero of $J_0$, the 4th zero of $J_2$, and
the 2nd zero of $J_7$. We can either find these by numerical methods, or else just look them up in a reference such as Abramowitz & Stegun where tables have been compiled. At any rate, their values are

\[
\begin{align*}
    z_{5,0} & \approx 14.9309 \\
    z_{4,2} & \approx 14.7960 \\
    z_{2,7} & \approx 14.8213
\end{align*}
\]

(It is not surprising that these values are so closely clustered; remember that $E_{n,l} \propto z_{n,l}^2$, so the energies of these states will also be very similar, which is the whole point.) So we can use a computer program such as Mathematica to plot the function

\[
f (\rho) = c_1 J_0^2 \left( 14.9309 \frac{\rho}{R} \right) + c_2 J_2^2 \left( 14.7960 \frac{\rho}{R} \right) + (1 - c_1 - c_2) J_7^2 \left( 14.8213 \frac{\rho}{R} \right)
\]

where we have put in coefficients $c_1$ and $c_2$ to allow us to give different weights to the various probability densities. It turns out, however, that the most naive choice we could make – giving all the states equal weights (i.e. $c_1 = c_2 = \frac{1}{3}$) – yields very reasonable results:

Looking at figure 2B in the paper, we see that we have reproduced the dotted theory line precisely; this line, in turn, tracks the solid data line very closely.