Particle in a box (also called an infinite square well) in 1D

Consider a quantum mechanical particle confined to \(0 < x < L\). One way to arrange this is with a potential energy

\[
V(x) = \begin{cases} 
0 & 0 < x < L \\
\infty & \text{otherwise}
\end{cases}
\]

Then, \(\Psi(x,t) = 0\) outside of \(0 < x < L\).

Inside of the one-dimensional box \(0 < x < L\), \(V(x) = 0\), so the time-independent Schrödinger equation

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

becomes

\[
-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2} \psi = 0.
\]

For \(E > 0\) it is convenient to define

\[
k = \sqrt{\frac{2mE}{\hbar^2}}.
\]

(We will see in problems in class and on the homework that there are no \(E \leq 0\) solutions satisfying the boundary conditions at \(x = 0\) and \(x = L\).) Then

\[
\frac{d^2\psi}{dx^2} + k^2 \psi = 0. \quad (1)
\]

Solutions: \((Recall\ simple\ harmonic\ oscillator\ from\ classical\ mechanics:\) ma = F_{spring} \Rightarrow m \frac{d^2x}{dt^2} = -k_{spring} x, \ \text{while} \ \omega = \sqrt{\frac{k_{spring}}{m}} \Rightarrow \frac{d^2x}{dt^2} + \omega^2 x = 0, \ \text{with} \ \text{solutions} \ x = A \sin \omega t + B \cos \omega t.)\)
Solutions to Eq. (1) are like those of a harmonic oscillator, except with \( x(t), \omega, t \rightarrow \psi(x), k, x \):

\[
\psi(x) = A \sin(kx) + B \cos(kx), \quad k = \sqrt{\frac{2mE}{\hbar^2}}.
\]

Boundary conditions (B.C.s) at \( x = 0 \) and \( x = L \):
\[
\psi(0) = \psi(L) = 0.
\]

\[
\psi(0) = 0 \implies A \sin(0) + B \cos(0) = 0, \quad \text{so} \ B = 0.
\]

\( \psi(x) \) is now \( \psi(x) = A \sin(kx) \).

Then,
\[
\psi(L) = 0 \implies A \sin(kL) = 0, \quad \text{so} \ kL = n\pi \]
\[
k_n = \frac{n\pi}{L}, \quad n = 1, 2, 3, \ldots.
\]

(n must be positive since \( k \) is positive.) Thus,

\[
\psi_n(x) = A_n \sin\left(\frac{n\pi x}{L}\right).
\]

(Solutions to time-indep. Schrödinger eq. for particle in a box.)

From \( k = \sqrt{\frac{2mE}{\hbar^2}} \) and \( k_n = \frac{n\pi}{L} \),

\[
E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \quad \text{(possible energies)}
\]

We have allowed for the possibility that the normalization constant might depend on \( n \), however, for this problem, it turns out that it doesn’t: \( A_n = \frac{\sqrt{2}}{L} \) independent of \( n \).

Including the time dependence:

\[
\psi_n(x,t) = \psi_n(x)e^{-i\frac{E_n t}{\hbar}}
\]

(Stationary states for particle in a box)
• Classically, a particle can bounce between the walls of the box with any energy $E$. Quantum mechanically, the boundary conditions are satisfied only for quantized (i.e., discrete) energies.

• For $n$th level, nodes at ends (from B.C.'s) and $(n-1)$ nodes in between. "integer number of $\frac{1}{2}$ wavelengths,"

$\psi_1(x)$  $\psi_2(x)$  $\psi_3(x)$

$n=1$  $n=2$  $n=3$

ground state  1st excited state  2nd excited state.

(Note, for other systems might have $n=0, 1, 2, \ldots$ instead of $n=1, 2, 3, \ldots$. Either way, used the terminology "ground state, 1st excited state, 2nd excited state, \ldots".)

• $\psi_n(x) = A_n \sin\left(\frac{n\pi x}{L}\right)$ is same shape as $n$th mode of a violin string. Same boundary conditions (fixed endpoints).

But, analogy stops there. Energy is $E_n = h\omega n$ for $n$th stationary state of a particle in a box. (Does not depend on amplitude $A_n$, which is fixed by normalization.) On the other hand, $E_{\text{violin}}$ depends on amplitude.

• Classically, $E=0$ is fine, but quantum mechanically there is no $E=0$ solution:

Node at each wall $\Rightarrow$ lowest energy $E_1 = \frac{\pi^2\hbar^2}{2mL^2}$

Interpretation: This is a consequence of Heisenberg's uncertainty principle, which says that a localized state
(wavefunction with a finite width \( \Delta x \)) must carry a range of momenta \( (\Delta p > 0) \) and therefore cannot be completely at rest (i.e., cannot be a state of definite momentum \( p = 0 \)).

\[
0 < x < L \Rightarrow \Delta x \leq L \quad (\frac{1}{\Delta x} \geq \frac{1}{L})
\]

\[
\Delta x \Delta p \geq \frac{\hbar}{2}
\]

\[
\Rightarrow \Delta p \geq \frac{\hbar}{2\Delta x} \geq \frac{\hbar}{2L}.
\]

Also,

\[
(\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2 = \langle p^2 \rangle \quad \text{turns out that} \quad \langle p \rangle = 0.
\]

(not surprising since box doesn't move)

So,

\[
\langle E \rangle = \frac{\langle p^2 \rangle}{2m} = \frac{(\Delta p)^2}{2m} = \frac{\hbar^2}{8mL^2}
\]

We expect that the actual ground state energy for a particle in a box won't be too different from the lower bound from the uncertainty principle. Very roughly then, we can estimate

\[
E_{\text{ground state}} \sim \frac{\hbar^2}{8mL^2}.
\]

This estimate is off only by \( 4\pi^2 \) from the exact result found above:

\[
E_1 = \frac{\pi^2 \hbar^2}{2mL^2} \quad \text{(from} \quad E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \text{)}.
\]
Discussion (continued)

- Why nodes for a particle bouncing back and forth in box? (Prob density $|\Psi|^2 = 0$ at node.) Answer:

$$\Psi_n(x,t) = \sqrt{\frac{2}{L}} \sin \left( \frac{n\pi x}{L} \right) e^{-i\frac{Et}{\sqrt{\omega_n}^2}}$$

$$= \sqrt{\frac{2}{L}} \frac{1}{2i} \left( e^{i(k_n x - \omega_n t)} - e^{-i(k_n x - \omega_n t)} \right), \quad k_n = \frac{n\pi}{L}.$$

- Moving in $+x$ direction, right-moving wave.
- Moving in $-x$ direction, left-moving wave.
- Right-moving and left-moving waves interfere.