In[143]:= Clear[n, m, a]
Particle in a 1-D box (con't)

What are expectation (average) values $<E>$, $<p>$, and $<x>$ when system is in stationary state $\psi_n(x)$?

1. $<a> = \frac{\int \psi_n \hat{A} \psi_n \, dx}{\int \psi_n \psi_n \, dx}$ so must know corresponding operators $\hat{A}$

2. $<a> = \text{eigenvalue of } \hat{A}$ only if $\psi_n = \text{eigenfunction of } \hat{A}$

3. $<a> \neq \text{eigenvalue of } \hat{A}$ if $\psi_n \neq \text{eigenfunction of } \hat{A}$

Rationale: If $\psi_n \neq \text{eigenfunction of } \hat{A}$, then $\psi_n$ can be written as a linear combination of mutually orthogonal eigenfunctions (see orthogonality & completeness theorems of Chapter 2). Integral shown in #1 above can be expanded in terms of these eigenfunctions, and leads to a weighted average of different eigenvalues rather than a single eigenvalue.

Suppose $\psi_n = \sum_{i=1}^{\infty} c_i f_i$ where $\hat{A} f_i = a_i f_i$ and $c_i = \text{constants}$

Then

$$<a> = \frac{\int (\sum_{i=1}^{\infty} c_i f_i) \hat{A} (\sum_{j=1}^{\infty} c_j f_j) \, dx}{\int (\sum_{i=1}^{\infty} c_i f_i) (\sum_{j=1}^{\infty} c_j f_j) \, dx}$$

Working on numerator only:

$$= \int (\sum_{i=1}^{\infty} c_i f_i) (\sum_{j=1}^{\infty} \hat{A} c_j f_j) \, dx = \int (\sum_{i=1}^{\infty} c_i f_i) (\sum_{j=1}^{\infty} a_j c_j f_j)$$

$$= \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} a_j c_i c_j \int f_i f_j \, dx = \sum_{i=1}^{\infty} a_i c_i^2$$

The final summation assumes the $f_i$ form an orthonormal set of functions (see Ch. 2)

Working on denominator gives same result without the $a_i$

$$= \int (\sum_{i=1}^{\infty} c_i f_i) (\sum_{m=1}^{\infty} c_m f_m) \, dx = \sum_{l=1}^{\infty} c_l^2$$

Combining it all gives:

$$<a> = \frac{\sum_{i=1}^{\infty} a_i c_i^2}{\sum_{l=1}^{\infty} c_l^2} = \text{weighted average of } a_i$$

This formula gives us a second definition of the expectation value that is consistent with the one given above. The first definition is more useful when we have a system's wave function and we know the relevant operator. The second definition is more useful when we know the eigenfunctions and eigenvalues of the operator and we know how to expand the wave function as a linear combination of eigenfunctions. In fact, we rarely have all of this information, so we mostly use the second definition to prove various theorems about expectation values.
\[ <E> = E_n \] because wave function is eigenfunction of \( \hat{H} \)

This just repeats what we stated above. Since \( \psi_n \) is an eigenfunction of \( \hat{H} \) the definition of \( <E> \) is also the formula for calculating \( E_n \).

\[ <p> \neq p_n \] because wave function is not eigenfunction of \( \hat{p} \)

Recall (Ch. 3) that \( \hat{p} = -i \hbar \frac{\partial}{\partial x} \). Following shows \( \hat{p} \psi \neq \text{const} \ast \psi \)

\[
\begin{align*}
\text{In}[144]:= & \quad -i \ast \hbar \ast \partial_x \left( \sqrt{\frac{2}{a}} \sin \left[ \frac{n \pi x}{a} \right] \right) \\
\text{Out}[144]= & \quad -i \sqrt{2} \left( \frac{1}{a} \right)^{3/2} \hbar n n \cos \left[ \frac{n \pi x}{a} \right]
\end{align*}
\]

Can use this result to calculate \( <p> \) (since wave function is normalized, we only need to calculate the numerator, \( \int \psi_n \hat{p} \psi_n \, dx \))

\[
\begin{align*}
\text{In}[159]:= & \quad \left[ \sqrt{\frac{2}{a}} \sin \left[ \frac{n \pi x}{a} \right] \right] (-i \ast \hbar) \ast \partial_x \left( \sqrt{\frac{2}{a}} \sin \left[ \frac{n \pi x}{a} \right] \right) \\
\text{Out}[159]= & \quad -2 i \hbar n \pi \cos \left[ \frac{n \pi x}{a} \right] \sin \left[ \frac{n \pi x}{a} \right] / a^2
\end{align*}
\]

\[
\begin{align*}
\text{In}[146]:= & \quad \int_{0}^{a} -2 i \hbar n \pi \cos \left[ \frac{n \pi x}{a} \right] \sin \left[ \frac{n \pi x}{a} \right] / a^2 \, dx \\
\text{Out}[146]= & \quad - \frac{i \hbar \sin \left[ n \pi \right]^2}{a}
\end{align*}
\]

\[
\begin{align*}
\text{In}[147]:= & \quad \text{Simplify}\left[ -\frac{i \hbar \sin \left[ n \pi \right]^2}{a}, \{ n \in \text{Integers} \} \right] \\
\text{Out}[147]= & \quad 0
\end{align*}
\]

Average value of momentum = 0, but average value is not eigenvalue of momentum. The particle may not actually be at rest (recall \( \text{KE} \neq 0 \)), and a single measurement of momentum on one system may not give \( p = 0 \).
\[ \langle x \rangle \neq x_n \text{ because wave function is not eigenfunction of } \hat{x} \]

Recall (Ch. 3) that \( \hat{x} = x \). Following shows \( \hat{x} \psi \neq \text{const} \psi \)

\[
\text{In}[148]:= \quad x \left( \sqrt{\frac{2}{a}} \sin \left[ \frac{n \pi x}{a} \right] \right)
\]

\[
\text{Out}[148]= \quad \sqrt{2} \sqrt{\frac{1}{a}} x \sin \left[ \frac{n \pi x}{a} \right]
\]

Can use this result to calculate \( \langle x \rangle \) (since wave function is normalized, we only need to calculate the numerator, \( \int \hat{x} \psi \psi \, dx \))

\[
\text{In}[149]:= \quad \left( \sqrt{\frac{2}{a}} \sin \left[ \frac{n \pi x}{a} \right] \right) \cdot \left( \sqrt{\frac{2}{a}} \sin \left[ \frac{n \pi x}{a} \right] \right)
\]

\[
\text{Out}[149]= \quad \frac{2 \sin \left[ \frac{n \pi x}{a} \right]^2}{a}
\]

\[
\text{In}[150]:= \quad \int_{0}^{a} \frac{2 \sin \left[ \frac{n \pi x}{a} \right]^2}{a} \, dx
\]

\[
\text{Out}[150]= \quad \frac{a (-1 - 2 n^2 \pi^2 + \cos(2 n \pi) + 2 n \pi \sin(2 n \pi))}{4 n^2 \pi^2}
\]

\[
\text{In}[151]:= \quad \text{Simplify} \left[ \frac{a (-1 - 2 n^2 \pi^2 + \cos(2 n \pi) + 2 n \pi \sin(2 n \pi))}{4 n^2 \pi^2}, \{ n \in \text{Integers} \} \right]
\]

\[
\text{Out}[151]= \quad \frac{\sqrt{2}}{2}
\]

Average position of particle is in middle of box for all quantum states.

Recall that \( P(a/2) \, dx \), the probability of finding particle near middle of box, changes with quantum state. Using \( P(a/2) \, dx = \psi(a/2)^2 \, dx \), I find:

\[
\text{In}[152]:= \quad \left( \sqrt{\frac{2}{a}} \sin \left[ \frac{n \pi (a/2)}{a} \right] \right) \cdot \left( \sqrt{\frac{2}{a}} \sin \left[ \frac{n \pi (a/2)}{a} \right] \right)
\]

\[
\text{Out}[152]= \quad \frac{2 \sin \left[ \frac{n \pi}{2} \right]^2}{a}
\]
In[153]:= 
Plot[2 Sin[\(\frac{n\pi}{2}\)]^2, \{n, 1, 6\}]

Out[153]=
- Graphics -

\(P(a/2)\) oscillates between large value & 0.

How do the probabilities of finding particle between 0→0.05\(a\) and 0.45\(a\)→0.5\(a\) behave?

In[154]:= 
\[P_{05} = \int_0^{0.05a} \left(\sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)\right) \left(\sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)\right) \, dx\]

\[P_{50} = \int_{0.45a}^{0.5a} \left(\sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)\right) \left(\sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)\right) \, dx\]

Out[154]=
0.05 - \(\frac{0.159155 \sin[0.314159 n]}{n}\)

Out[155]=
\(\frac{1}{n} \left(0.05 \, n + 0.159155 \sin[2.82743 \, n] - 0.159155 \sin[3.14159 \, n]\right)\)
Recap

Measurement produces eigenvalue of $\hat{A}$ if made only once
- does not require $\psi$ to be eigenfunction of $\hat{A}$
- if $\psi$ = e-fn, then observe e-value of this e-fn
- if $\psi \neq$ e-fn, then result is unpredictable, but can obtain rel. probabilities of different results by expanding $\psi$ as linear combination of e-fns

Measurement produces expectation value $<a>$ if repeated on many identical systems
- does not require $\psi$ to be eigenfunction of $\hat{A}$
- if $\psi$ = e-fn, then $<a>$ = e-value of this e-fn
- if $\psi \neq$ e-fn, then result obtained from $\int \psi \hat{A} \psi \, dx$

Probability of finding particle at $x \neq <\chi>$
- $<\chi> = \int \psi \hat{A} \psi \, dx$
- $P(x) = \psi^2$