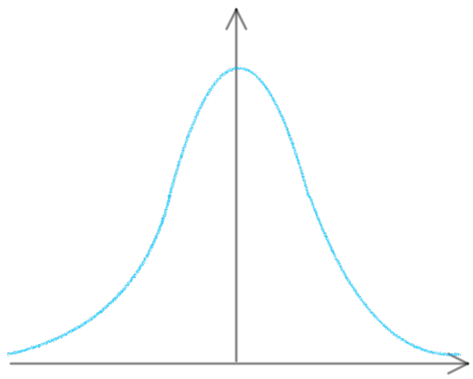
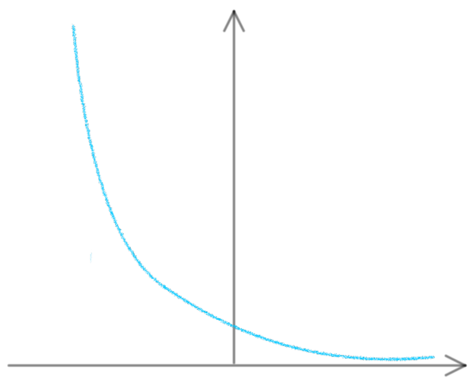
QMS Problem Set 1

W1: Plotting the functions with $a=1$



$f(x) = e^{-x^2}$



$f(x) = e^{-x}$

- From the plots we can see that e^{-ax^2} can be normalized and e^{-ax} cannot
- Hence e^{-ax} is not an acceptable wf
- e^{-ax^2} can be an acceptable wave function
  - it has finite values and hence finite integral (Born interpretation)
  - it is single-valued and continuous
  - it has a continuous first derivative (exponential function)
    = it can be derived twice

W 2: Operating with $\frac{d}{dx}$

i) $\frac{d}{dx} \cos(kx) = -k \sin(kx)$ || not an eigenfunction

ii) $\frac{d}{dx} e^{ikx} = ik\, e^{ikx}$ || eigenfunction with eigenvalue ik

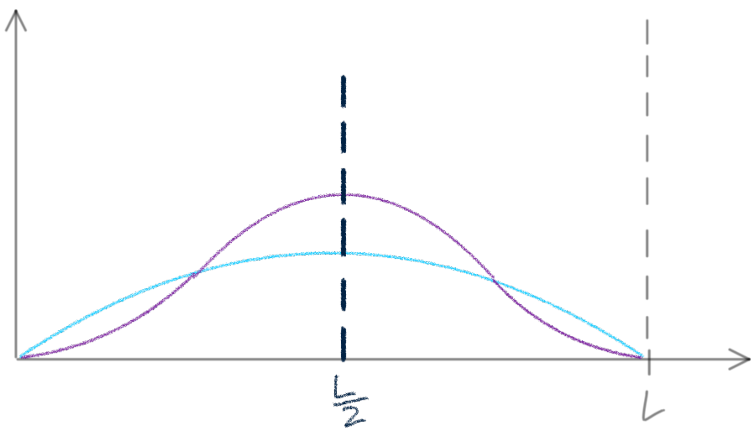
iii) $\frac{d}{dx} kx = k$ || not an eigenfunction

iv) $\frac{d}{dx} e^{-ax^2} = -2ax\, e^{-ax^2}$ || not an eigenfunction because $-2ax$ is not constant

W3: The particle in a box $n=1$

Wave function $\psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)$

Probability density $|\psi_1|^2(x) = \frac{2}{L} \sin^2\left(\frac{\pi x}{L}\right)$



The expectation value of x marked: $\langle x \rangle$ tells the average value of x in multiple measurements done on identical systems.

The probability density is symmetrical so it is equally likely to find the particle on either side of $\frac{L}{2}$. Thus the measurements average to $\frac{L}{2}$

P1: Normalization ensures that the wave function complies to the Born interpretation.

Born interpretation states that the probability of finding the particle with wf ψ is proportional to $|\psi^2|dx$.

Consider the whole volume where ψ can exist:

- finding the particle inside is certain

$\Rightarrow P(\text{find particle}) = 1 = 100\%$

Hence $\int_\tau |\psi|^2 d\tau = 1$

Normalization of the wave function ensures that the condition $\int_\tau |\psi|^2 d\tau = 1$ holds.

With this exercise I am using Mathematica

There's Wolfram Alpha and others online.

A free particle with wavefunction $\psi(x) = e^{-ax^2}$

$a = 0.2 \frac{1}{m^2}$

The wavefunction is unnormalized so

let's normalize it first:

In[1]:= **Integrate e^(-0.2*2x^2) from -infty to infty**

Definite integral:

$$\int_{-\infty}^{\infty} e^{-0.2\times 2 x^2}\, dx = 2.8025$$

Then let's calculate the integral when

$x \geq 1\,m$

In[3]:= **Integrate 1/(2.8025) e^(-0.2*2x^2) from 1 to infty**

Definite integral:

$$\int_{1}^{\infty} \frac{e^{-0.2\times 2 x^2}}{2.8025}\, dx = 0.185546$$

The value from the integral is the probability: ≈18.6%

P2: The value of a commutator essentially implies if the order of the two operations matter: $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

- If the value is zero then there's no difference between $\hat{A}\hat{B}$ and $\hat{B}\hat{A}$

Another point of view:

If two operators commute they have the same set of eigenfunctions!

- As the function does not change in the operation $\hat{A} f(x)$ or $\hat{B} f(x)$ then the order of operations does not matter

In Quantum Mechanics (QM) relate to the Heisenberg's uncertainty principle:

- If two operators do not commute, then the corresponding obervables cannot be known simultaneously with an arbitrary precision

In short:

$[\hat{A},\hat{B}]=0 \longrightarrow$ no problems there

$[\hat{A},\hat{B}]\neq 0 \longrightarrow$ the uncertainty principle

i) $[\hat{H},\hat{p}_x]$ where $V(x)=V_0$

$= \hat{H}\hat{p}_x\psi - \hat{p}_x\hat{H}\psi$ || I use ψ as a "dummy function"

$$=\left(\frac{\hat{p}_x^2}{2m}+V_0\right)\hat{p}_x\psi - \hat{p}_x\left(\frac{\hat{p}_x^2}{2m}+V_0\right)\psi$$

$$=\frac{\hat{p}_x^2}{2m}\hat{p}_x\psi + V_0\hat{p}_x\psi - \hat{p}_x\frac{\hat{p}_x^2}{2m}\psi - \hat{p}_x(V_0\psi)$$

$$=\frac{\hat{p}_x^3}{2m}\psi + V_0\hat{p}_x\psi - \frac{\hat{p}_x^3}{2m}\psi - V_0\hat{p}_x\psi$$

$=0$

ii) $[\hat{H}, \hat{p}_x]$ where $V(x) = \frac{1}{2} k_f x^2$

$$= \hat{H}\hat{p}_x \psi - \hat{p}_x \hat{H} \psi$$

product rule of derivatives

$$= \left(\frac{\hat{p}_x^2}{2m} + \frac{1}{2} k_f x^2\right) \hat{p}_x \psi - \hat{p}_x \left(\frac{\hat{p}_x^2}{2m} + \frac{1}{2} k_f x^2\right) \psi$$

$$= \frac{\hat{p}_x^2}{2m} \hat{p}_x \psi + \frac{1}{2} k_f x^2 \hat{p}_x \psi - \hat{p}_x \frac{\hat{p}_x^2}{2m} \psi - \hat{p}_x \left(\frac{1}{2} k_f x^2 \psi\right)$$

$$= \frac{\hat{p}_x^3}{2m} \psi + \frac{1}{2} k_f x^2 \hat{p}_x \psi - \frac{\hat{p}_x^3}{2m} \psi - \left[\frac{1}{2} k_f x^2 \hat{p}_x \psi + \psi \hat{p}_x \left(\frac{1}{2} k_f x^2\right)\right]$$

$$= - \psi \hat{p}_x \left(\frac{1}{2} k_f x^2\right)$$

// Remove the dummy function

// $\hat{p}_x = -i\hbar \frac{d}{dx}$

$$= -i\hbar \left(-k_f x\right)$$

$$= i\hbar k_f x$$

P3: a/ The probability densities for all particle in a box wavefunctions are symmetrical in relation to $\frac{L}{2}$. Therefore particle position measurements result on average to $\frac{L}{2}$

b) There's two options for the particle to move: positive x direction or negative x direction. If the probabilities for both directions match (ie. 50:50) then the results of momentum measurements average to zero.

Turns out they do match:

The particle in a box wavefunction is a superposition $\left[\Psi = c_1 \Psi_1 + c_2 \Psi + \ldots\right]$ of two momentum operator eigenfunctions:

$$\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) = \sqrt{\frac{2}{L}} \; \frac{e^{\left(\frac{in\pi x}{L}\right)} - e^{\left(\frac{-in\pi x}{L}\right)}}{2i}$$

The superposition coefficients $c_1, c_2, \ldots$ squared $|c_n|^2$ are proportional to the probability of ψ_n emerging from the measurement.

c) $\langle x^2 \rangle = \int_\tau \psi^* x^2 \psi \, d\tau$

For a particle in a box of length L the whole space is essentially $x \in [0, L]$

$$\langle x^2 \rangle = \frac{2}{L} \int_0^L \sin\left(\frac{n\pi x}{L}\right) x^2 \sin\left(\frac{n\pi x}{L}\right) dx$$

$$\langle x^2 \rangle = \frac{2}{L} \int_0^L x^2 \sin^2\left(\frac{n\pi x}{L}\right) dx$$

Use the formula from Atkins' Resources on Tables.pdf in MyC

$$\langle x^2 \rangle = \frac{2}{L}\left[\frac{L^3}{6} - \left(\frac{L^2}{4\left(\frac{n\pi}{L}\right)} - \frac{1}{8\left(\frac{n\pi}{L}\right)^3}\right)\sin\left(\frac{2n\pi}{L}L\right) - \frac{L}{4\left(\frac{n\pi}{L}\right)^2}\cos\left(\frac{2n\pi}{L}L\right)\right]$$

$$\langle x^2 \rangle = \frac{2}{L}\left[\frac{L^3}{6} - \left(\frac{L^3}{4n\pi} - \frac{L^3}{8n^3\pi^3}\right)\sin(2n\pi) - \frac{L^3}{4n^2\pi^2}\cos(2n\pi)\right]$$

$$\langle x^2 \rangle = \left[\frac{L^2}{3} - \left(\frac{L^2}{2n\pi} - \frac{L^2}{4n^3\pi^3}\right)\underbrace{\sin(2n\pi)}_{\text{always } 0} - \frac{L^2}{2n^2\pi^2}\underbrace{\cos(2n\pi)}_{\text{always } 1}\right]$$

$$\langle x^2 \rangle = \frac{L^2}{3} - \frac{L^2}{2n^2\pi^2}$$

$$\langle x^2 \rangle = L^2\left(\frac{1}{3} - \frac{1}{2n^2\pi^2}\right)$$

d) Classically energy and momentum are linked by formula $E = \frac{p^2}{2m}$ where p = momentum and m = mass

That holds true also in quantum mechanics and kinetic energy operator can be written as $\hat{K} = \frac{\hat{p}^2}{2m}$

Recall that in the box all energy is kinetic and hence the Hamiltonian is $\hat{H} = \frac{\hat{p}_x^2}{2m}$ as well.

Now the WF of the system must be an eigenfunction of $\hat{p}_x^2$ as well ie. $[\hat{H}, p_x^2] = 0$

Thus the only possible result for measurement of $\hat{p}_x^2$ is the eigenvalue of $\hat{p}_x^2$ which can be calculated from the energy eigenvalue:

$$\langle p_x^2 \rangle = 2m \cdot \frac{n^2 h^2}{8mL^2} = \frac{n^2 h^2}{4L^2}$$

Bonus:

a/ $\langle x \rangle = \frac{L}{2}$ $\langle x^2 \rangle = L^2\left(\frac{1}{3} - \frac{1}{2n^2\pi^2}\right)$

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

$$\Delta x = \sqrt{L^2\left(\frac{1}{3} - \frac{1}{2n^2\pi^2}\right) - \left(\frac{L}{2}\right)^2}$$

$$\Delta x = \sqrt{\frac{L^2}{3} - \frac{L^2}{2n^2\pi^2} - \frac{L^2}{4}}$$

$$\Delta x = \sqrt{\frac{L^2}{12} - \frac{L^2}{2n^2\pi^2}}$$

$$\Delta x = L\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}}$$

$\langle p_x \rangle = 0$ $\langle p_x^2 \rangle = \frac{n^2h^2}{4L^2}$

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$$

$$\Delta p = \sqrt{\frac{n^2h^2}{4L^2} - 0^2}$$

$$\Delta p = \sqrt{\frac{n^2h^2}{4L^2}}$$

$$\Delta p = \frac{nh}{2L}$$

b)

$$\Delta x \Delta p = L\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}}\left(\frac{nh}{2L}\right)$$

$$\Delta x \Delta p = \frac{nh}{2}\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}}$$

$$\Delta x \Delta p = \frac{nh}{2}\sqrt{\frac{2n^2\pi^2}{24n^2\pi^2} - \frac{12}{24n^2\pi^2}}$$

$$\Delta x \Delta p = \frac{nh}{2}\sqrt{\frac{2n^2\pi^2 - 12}{24n^2\pi^2}}$$

$$\Delta x \Delta p = \sqrt{\frac{n^2h^2}{4}\,\frac{2n^2\pi^2 - 12}{24n^2\pi^2}}$$

$$\Delta x \Delta p = \sqrt{\frac{h^2}{4}\,\frac{2n^2\pi^2 - 12}{24\pi^2}}$$

$$\Delta x \Delta p = \sqrt{\frac{h^2}{4}\,\frac{2n^2\pi^2 - 12}{6(2\pi)^2}}$$

$$\Delta x \Delta p = \sqrt{\frac{\hbar^2}{4}\,\frac{2n^2\pi^2 - 12}{6}}$$

$$\Delta x \Delta p = \frac{\hbar}{2}\sqrt{\frac{n^2\pi^2 - 6}{3}}$$

c/ Heisenberg's uncertainty principle states that $\Delta x \Delta p \geq \frac{\hbar}{2}$

For $n=1$ $\Delta x \Delta p = \frac{\hbar}{2}\sqrt{\frac{\pi^2 - 6}{3}} \geq \frac{\hbar}{2}$

For $n=2$ $\Delta x \Delta p = \frac{\hbar}{2}\sqrt{\frac{4\pi^2 - 6}{3}} \geq \frac{\hbar}{2}$

As $n^2\pi^2 > 6$ always, thus $\frac{\hbar}{2}\sqrt{\frac{n^2\pi^2 - 6}{3}} \geq \frac{\hbar}{2}$

holds for $n \geq 1$