A short refresher on probability

If a discrete variable j takes a total of N values, the probability of value j is

$$P(j) = \frac{N(j)}{N}$$ where $N(j)$ is number of instances of j

Observe that ① $\sum_j P(j) = 1$

② Average of j, $\langle j \rangle = \frac{\sum j N(j)}{N} = \sum_j j P(j)$

③ For any function $f(j)$, $\langle f(j) \rangle = \sum_j f(j) P(j)$

For continuous variables,

$$P_{ab} = \int_a^b \rho(x)\, dx$$ where $\rho(x)\, dx$ is the probability that a chosen value of x lies between x and $x + \Delta x$

Then, $$\int_{-\infty}^{\infty} \rho(x)\, dx = 1$$

$$\langle x \rangle = \int_{-\infty}^{\infty} x \rho(x)\, dx$$

$$\langle f(x) = \int_{-\infty}^{\infty} f(x) \rho(x)\, dx$$

Expetation value of position of a quantum particle

From Born's statistical interpretation, for a particle in state $\psi(x,t)$, the probability of finding it at x is

$$\rho(x) = |\psi(x,t)|^2$$

And the expetation value of x is

$$\langle x \rangle = \int_{-\infty}^{\infty} x \rho(x)\, dx$$

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x,t)|^2\, dx$$

$\langle x \rangle$ gives the average of measurements of position on an ~~ensamble~~ ensable of identically prepared systems.

Expetation value of momentum of a quantum particle

$$p = mv = m \frac{dx}{dt}$$

$$\langle p \rangle = m \frac{d\langle x \rangle}{dt}$$

or $\langle p \rangle = m \frac{d}{dt} \int_{-\infty}^{\infty} x |\psi|^2 dx$

or $\langle p \rangle = m \int_{-\infty}^{\infty} x \frac{\partial}{\partial t} |\psi|^2 \, dx$

Now, for a moment, consider $\frac{\partial}{\partial t} |\psi|^2$

$$\frac{\partial}{\partial t} |\psi|^2 = \frac{\partial}{\partial t} (\psi^* \psi) = \psi \frac{\partial \psi^*}{\partial t} + \frac{\partial \psi}{\partial t} \psi^*$$

Schrödinger equation is

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi$$

or $$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} - \frac{i}{\hbar} V \psi \quad \text{—— (3.1)}$$

Taking complex conjugate

$$\frac{\partial \psi^*}{\partial t} = -\frac{i\hbar}{2m} \frac{\partial^2 \psi^*}{\partial x^2} + \frac{i}{\hbar} V\psi \quad \text{—— (3.2)}$$

upon $\psi^* \times$ eq (3.1) + $\psi \times$ eq (3.2)

$$\psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t} = \frac{i\hbar}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi^*}{\partial x^2} \right]$$

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

(Hint: applying product rule in the latter will lead to former)

Now, substituting for $\frac{\partial}{\partial t}|\psi|^2$

$$\langle p \rangle = m \int_{-\infty}^{\infty} x \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right)\right]$$

$$= \frac{i\hbar}{2}\int_{-\infty}^{\infty} x \frac{\partial}{\partial x}\left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right) dx$$

Integration-by-parts note

$$\frac{d}{dx}(uv) = u\frac{dv}{dx} + \frac{du}{dx}v$$

Integrating both sides w.r.t x between a and b

$$uv\Big|_a^b = \int_a^b u\frac{dv}{dx}\,dx + \int_a^b \frac{du}{dx}v\,dx$$

or $$\int_a^b u\frac{dv}{dx}\,dx = -\int_a^b \frac{du}{dx}v\,dx + uv\Big|_a^b$$

Returning to $\langle p \rangle$

$$\langle p \rangle = -\frac{i\hbar}{2}\int_{-\infty}^{\infty}\frac{dx}{dx}\cdot\left(\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right)dx \quad \cancel{\text{constant}} \; 0 \text{ at } \infty$$

$$= -\frac{i\hbar}{2}\int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\,dx$$

Reapplying the same trick again, $\langle p \rangle = -\frac{i\hbar}{2}\int_{-\infty}^{\infty} 2\psi^*\frac{\partial\psi}{\partial x}\,dx$

So, $\boxed{\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x}\, dx}$

Operator formalism

$$\langle x \rangle = \int_{-\infty}^{\infty} x\, |\psi(x,t)|^2\, dx \quad \text{(as we derived previously)}$$

$$= \int_{-\infty}^{\infty} \psi^* \, x \, \psi \, dx$$

$$= \int_{-\infty}^{\infty} \psi^* \, \hat{x} \, \psi \, dx$$ where $\hat{x}$ is position operator, $\hat{x} = x$

$$\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x}\, dx \quad \text{(as we derived previously)}$$

$$= \int_{-\infty}^{\infty} \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \psi \, dx$$

$$= \int_{-\infty}^{\infty} \psi^* \, \hat{p} \, \psi \, dx$$ where $\hat{p}$ is the momentum operator, $\hat{p} = -i\hbar \frac{\partial}{\partial x}$

Since, $\hat{T} = \frac{\hat{p}^2}{2m} = \frac{1}{2m}\left(-i\hbar \frac{\partial}{\partial x}\right)^2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

$$\langle T \rangle = \int_{-\infty}^{\infty} \psi^* \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right) \psi \, dx$$

Heisenberg Uncertainty Principle

$$\sigma_x \cdot \sigma_p \geq \hbar/2$$

where $\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2$ is variance in the measurement of x

$\sigma_p^2 = \langle p^2 \rangle - \langle p \rangle^2$ is the variance in the measurement of p

Q. A particle of mass m has the wave function

$$\Psi(x,t) = A e^{-a[(mx^2/\hbar) + it]}$$

where A and a are real positive constants.

ⓐ Find A.

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \, dx = 1$$

or $$A^2 \int_{-\infty}^{\infty} e^{-2amx^2/\hbar} \, dx = 1$$

Recall $$\int_{-\infty}^{\infty} e^{-x^2/a^2} \, dx = a\sqrt{\pi}$$

So, $$A^2 \int_{-\infty}^{\infty} e^{-x^2/\left(\sqrt{\frac{\hbar}{2am}}\right)^2} \, dx = 1$$

or $$A^2 \sqrt{\frac{\hbar}{2am}} \cdot \sqrt{\pi} = 1$$

or $$A^2 \sqrt{\frac{\hbar\pi}{2am}} = 1$$

$$\therefore A = \sqrt[4]{\frac{2am}{\hbar\pi}}$$

So, the wave function is $\Psi(x,t) = \sqrt[4]{\frac{2am}{\hbar\pi}} \, e^{-a\left[\frac{mx^2}{\hbar} + it\right]}$

(b)

For what potential energy function, $V(x)$, is this a solution to the Schrödinger's equation?

Recall Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi$$

$$\text{or } V = \frac{1}{\psi}\left[i\hbar \frac{\partial \psi}{\partial t} + \frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \right]$$

$$\text{or } V = \frac{1}{\psi}\left[i\hbar \left(\frac{2am}{\pi\hbar}\right)^{\frac{1}{4}} e^{-a\left[\frac{mx^2}{\hbar}+it\right]} \cdot (-ia) + \frac{\hbar^2}{2m}\left(\frac{2am}{\pi\hbar}\right)^{\frac{1}{4}} \frac{\partial}{\partial x}\left(e^{-a\left(\frac{mx^2}{\hbar}+it\right)} \cdot \left(-\frac{2amx}{\hbar}\right)\right)\right]$$

$$\text{or } V = \frac{1}{\psi}\left[i\hbar \cdot \psi \cdot (-ia) + \frac{\hbar^2}{2m}\left(\frac{2am}{\pi\hbar}\right)^{\frac{1}{4}} \left\{ -\frac{2am}{\hbar} \left(e^{-a\left(\frac{mx^2}{\hbar}+it\right)} + x e^{-a\left(\frac{mx^2}{\hbar}+it\right)} \cdot \left(-\frac{2amx}{\hbar}\right)\right)\right\}\right]$$

$$\text{or } V = \frac{1}{\psi}\left[\hbar a\psi + \frac{\hbar^2}{2m}\left(-\frac{2am}{\hbar}\right)\psi + \frac{\hbar^2}{2m}\psi \frac{4a^2m^2x^2}{\hbar^2} \right]$$

$$V = \hbar a - \hbar a + 2ma^2x^2$$

$$\therefore V = 2ma^2x^2$$

(c) Calculate the expectation values of x, x^2, p and p^2

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^* x \psi \, dx$$

$$= \int_{-\infty}^{\infty} \sqrt[4]{\frac{2am}{\pi\hbar}} e^{-a\left(\frac{mx^2}{\hbar} - it\right)} \cdot x \cdot \sqrt[4]{\frac{2am}{\pi\hbar}} e^{-a\left(\frac{mx^2}{\hbar} + it\right)} dx$$

$$= \sqrt{\frac{2am}{\pi\hbar}} \int_{-\infty}^{\infty} x e^{-2amx^2/\hbar} dx$$

Integral of an ~~od~~ odd function over symmetric limit is zero

so, $\langle x \rangle = 0$

$$\langle x^2 \rangle = \int \psi^* x^2 \psi \, dx$$

$$= \sqrt{\frac{2am}{\pi\hbar}} \int_{-\infty}^{\infty} x^2 e^{-2amx^2\hbar} dx$$

$$\langle x^2 \rangle = \sqrt{\frac{2am}{\pi\hbar}} \int_{-\infty}^{\infty} x^2 e^{-x^2/\left(\sqrt{\hbar/2am}\right)^2} dx$$

Using $\displaystyle\int_{-\infty}^{\infty} x^2 e^{-x^2/a^2} dx = \frac{a^3\sqrt{\pi}}{2}$

$$\langle x^2 \rangle = \sqrt{\frac{2am}{\pi\hbar}} \left(\frac{\hbar}{2am}\right)^{3/2} \frac{\sqrt{\pi}}{2} = \frac{\hbar}{4am}$$

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^* \left(-i\hbar\frac{\partial}{\partial x}\right) \psi \, dx$$

$$= \sqrt{\frac{2am}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-a\left(\frac{mx^2}{\hbar} - it\right)} \cdot (-i\hbar) \cdot \frac{\partial}{\partial x}\left(e^{-a\left(\frac{mx^2}{\hbar} + it\right)}\right) dx$$

$$= \sqrt{\frac{2am}{\pi\hbar}} (-i\hbar) \int_{-\infty}^{\infty} e^{-a\left(\frac{mx^2}{\hbar} - it\right)} \cdot e^{-a\left(\frac{mx^2}{\hbar} + it\right)} \cdot \left(-\frac{2amx}{\hbar}\right) dx$$

$$= i \cdot 2am \cdot \sqrt{\frac{2am}{\pi\hbar}} \underbrace{\int_{-\infty}^{\infty} x e^{-2amx^2/\hbar} dx}_{= 0 \ (\because \text{ odd function})}$$

$$= 0$$

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right)^2 \psi \, dx$$

$$= -\hbar^2 \sqrt{\frac{2am}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-a\left(\frac{mx^2}{\hbar} - it\right)} \frac{\partial^2}{\partial x^2}\left[e^{-a\left(\frac{mx^2}{\hbar} + it\right)}\right] dx$$

Solve ______

use $\int_{-\infty}^{\infty} e^{-x^2/a^2} = a\sqrt{\pi}$

$\int_{-\infty}^{\infty} x^2 e^{-x^2/a^2} = \frac{a^3\sqrt{\pi}}{2}$

$$\langle p^2 \rangle = \hbar a m$$

(d) Find σ_x and σ_p. Is their product consistent with Heisenberg uncertainty principle.

$$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\frac{\hbar}{4am} - 0} = \frac{1}{2}\sqrt{\hbar/am}$$

$$\sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\hbar a m - 0} = \sqrt{\hbar a m}$$

$$\sigma_x \cdot \sigma_p = \frac{1}{2}\sqrt{\frac{\hbar}{am}} \cdot \sqrt{\hbar a m} = \hbar/2$$

Yes, it is consistent.