1/12/04

Lecture 3 Gaussian Integrals

Would like to calculate

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

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} dx\, x^2\, \Psi^* \Psi$$

and

$$\Delta x = \left[\langle x^2 \rangle - \langle x \rangle^2 \right]^{1/2} \quad \text{uncert.}$$

for various wave functions $\Psi = \Psi(x,t)$

Note wave functions in QM are complex

$$\Psi = \mathrm{Re}\,\Psi + i\,\mathrm{Im}\,\Psi$$

$$i = \sqrt{-1}, \quad i^2 = -1, \quad 1/i = -i$$

Complex conjugate of $\Psi \equiv \Psi^*$

$$\Psi^* = \mathrm{Re}\,\Psi - i\,\mathrm{Im}\,\Psi, \quad (i \to -i)$$

$$|\Psi|^2 \equiv \Psi^* \Psi = (\mathrm{Re}\,\Psi + i\,\mathrm{Im}\,\Psi)(\mathrm{Re}\,\Psi - i\,\mathrm{Im}\,\Psi)$$

$$= (\mathrm{Re}\,\Psi)^2 - i^2 (\mathrm{Im}\,\Psi)^2 = (\mathrm{Re}\,\Psi)^2 + (\mathrm{Im}\,\Psi)^2 \geq 0$$

Prob. density $\rho(x,t) \equiv \Psi^* \Psi$

Important example: <u>Gaussian</u> wave functions

Function is called a gaussian if it involves any combination of e^{x^2}

$$e^{-\lambda (x - x_0)^2}, \quad e^{-\frac{1}{2}\left(\frac{x}{\sigma}\right)^2} \quad \ldots$$

Interested in integrals of the form

$$I_n = \int_{-\infty}^{\infty} dx\, e^{-x^2}\, x^n$$

$\langle x \rangle \longleftrightarrow I_1 \qquad \langle x^2 \rangle \longleftrightarrow I_2$

etc. if $\Psi = A e^{-\frac{x^2}{2}}$

A is normalization

$$\Psi^* \Psi = A^* A\, e^{-x^2}$$

$$\int_{-\infty}^{\infty} A^* A\, e^{-x^2} dx = \int_{-\infty} dx\, \Psi^* \Psi = 1$$

$$A^* A = 1 \Big/ \int_{-\infty}^{\infty} e^{-x^2} dx$$

First need $I_0 = \int_{-\infty}^{\infty} e^{-x^2} dx$

Note $\Psi = A\, e^{-x^2/2}$ so $\rho = \Psi^* \Psi = A^* A\, e^{-x^2}$

There is a special trick to evaluate I_0

$$I_0\, I_0 = \left[\int_{-\infty}^{\infty} dx\, e^{-x^2}\right]\left[\int_{-\infty}^{\infty} dy\, e^{-y^2}\right] = I_0^2$$

let $r^2 = x^2 + y^2$ change of variables

$$x = r\cos\phi \qquad y = r\sin\phi$$

$$dx\, dy = r\, dr\, d\phi$$

In general change of variables

$$dx\, dy = \begin{vmatrix} \frac{dx}{dr} & \frac{dx}{d\phi} \\ \frac{dy}{dr} & \frac{dy}{d\phi} \end{vmatrix} dr\, d\phi$$

$$\frac{\partial x}{\partial r} = \cos\phi \qquad \frac{\partial x}{\partial \phi} = -r\sin\phi$$

$$\frac{\partial y}{\partial r} = \sin\phi \qquad \frac{\partial y}{\partial \phi} = r\cos\phi$$

$$I_0^2 = \int_0^\infty r\,dr \int_0^{2\pi} d\phi \; e^{-r^2} = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \; e^{-x^2+y^2}$$

$$\int_0^{2\pi} d\phi = 2\pi$$

$$\int_0^\infty r\,dr\, e^{-r^2} = \int_0^\infty \frac{dt}{2}\, e^{-t} \qquad t = x^2 = r^2$$

$$dt = 2x\,dx = 2r\,dr$$

$$= \frac{1}{2}\left(-e^{-t}\right)\Big|_0^\infty = \frac{1}{2}$$

$$I_0^2 = \frac{1}{2}\, 2\pi = \pi$$

$$I_0 = \boxed{\int_{-\infty}^{\infty} dx\, e^{-x^2} = \pi^{1/2}}$$

Now consider I_1

$$I_1 = \int_{-\infty}^{\infty} dx \;\; x e^{-x^2} = \int_{-\infty}^{\infty} dx \;\; f(x)$$

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

Integral of any odd function of x from $-\infty$ to ∞ is zero

odd function $\qquad f(x) = -f(-x)$

$$\int_{-\infty}^{\infty} dx\, f(x) = \int_0^\infty dx\, f(x) + \int_{-\infty}^0 dx\, f(x)$$

let $y = -x$ in 2nd integral

$$\int_{-\infty}^0 dx\, f(x) = -\int_\infty^0 dy\, f(-y) = \int_0^\infty dy\, f(-y)$$

Now $f(-y) = -f(y)$

so $\int_{-\infty}^{0} dx\, f(x) = -\int_{0}^{\infty} dy\, f(y)$

change dummy variable back $x = y$

$$= -\int_{0}^{\infty} dx\, f(x)$$

$$\int_{-\infty}^{\infty} dx\, f(x) = \int_{0}^{\infty} dx\, f(x) - \int_{0}^{\infty} dx\, f(x) = 0$$

all odd integrands vanish

$I_n = 0$ for n odd.

What about

$$I_2 = \int_{-\infty}^{\infty} dx\, x^2 e^{-x^2}$$

Use integration by parts to relate it to I_0

Integration by parts

$$\int_a^b dV\, U = -\int_a^b dU\, V + \underbrace{UV\Big|_a^b}_{\text{contribution from end points}}$$

Let $dV = x\,dx\,e^{-x^2}$ $\qquad U = x$

$V = -\frac{1}{2}e^{-x^2}$ $\qquad dU = dx$

$$\int_{-\infty}^{\infty} dV\, U = \int_{-\infty}^{\infty} dx\, x\, e^{-x^2} x = I_2$$

$$= -\int dU\, V + UV\Big|_{-\infty}^{\infty}$$

$$= -\int_{-\infty}^{\infty} dx \left(\frac{-1}{2}\right) e^{-x^2} + -\frac{x}{2} e^{-x^2}\Big|_{-\infty}^{\infty}$$

$$= \frac{1}{2} \int_{-\infty}^{\infty} dx\, e^{-x^2} + 0 = \frac{1}{2} I_0$$

$$\boxed{I_2 = \int_{-\infty}^{\infty} dx\, x^2 e^{-x^2} = \frac{1}{2} \pi^{1/2}}$$

Can keep going to relate I_4 to I_2 and I_6 to I_4 ...

This will allow you to do all integrals needed for prob. 1.6

Schrodinger Eq.

How does wave function evolve in time $\Rightarrow$ it spreads

How do particles move in classical mechanics? Newton's 2nd law

$$F = ma$$

$$\Rightarrow \ddot{x} = \frac{1}{m} F$$

In quantum mechanics

$$\boxed{i\hbar \frac{\partial \Psi}{\partial t}(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi(x,t)}$$

This is Schrodinger eq.
We have not derived it! can take it as a basic postulate of QM
Just like we did not derive Newton's 2nd law.

So QM deals with a wave function $\Psi(x,t)$ ~~wh~~ wich describe system (in this case one particle constrained to move in 1 dim.)

Meaning of wave function

$$\rho(x,t) = \Psi^*(x,t)\,\Psi(x,t) \geq 0$$

is prob. density to find particle at x
Prob. must be normalized.

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

Important consistency check. If Ψ is normalized at $t=0$ will it stay normalized if it evolves according to S. eq?