FI-I

Fourier Integrals and Dirac Delta Function

Anatoliy introduced the complex form of Fourier series.

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{in x\pi/L} \qquad c_n = \frac{1}{2L}\int_{-L}^{L} f(x)\, e^{-inx\pi/L}\, dx$$

integers.

NOTE: CORRECTION TO NOTES.

We have discussed how the collection of continuous functions on an interval forms a vector space and that the numbers $f(x)$ can be viewed as the components of f, commenting on analogies like

$$\vec{v}\cdot\vec{w} = v_1^* w_1 + v_2^* w_2 + v_3^* w_3$$

$$\Longleftrightarrow \quad f\cdot g = \int dx\, f^*(x)\, g(x) \qquad \text{etc.}$$

We also noted that the Fourier coefficients can be viewed as the components of f in the new basis of $\sin\frac{n\pi x}{L}$, $\cos\frac{n\pi x}{L}$ (or $e^{in\pi x/L}$) which form a complete set.

There is something a bit odd about this.

For conventional vectors in real space we have 3 components and if we change basis we still have 3 components. Here in our original bases f has a continuous infinity of components $f(x)$ (real) while in the new Fourier bases a discrete infinity. c_n (n integer)

This asymmetry is reflected in the transformation eqns $f(x) \Leftrightarrow c_n$ which look dissimilar:

This lack of symmetry goes away if we consider the limit $L \to \infty$ (and hence consider general functions f, not just periodic ones)

Let's first note that in the relations between $f(x)$ and c_n we can place the prefactors wherever we like

$$f(x) = \sum_{-\infty}^{\infty} c_n e^{in\pi/L\, x} \qquad c_n = \frac{1}{2L}\int_{-L}^{L} f(x) e^{-\frac{in\pi}{L}x}\, dx$$

$$\Longleftrightarrow \quad f(x) = \frac{1}{2L}\sum_{-\infty}^{\infty} c_n e^{in\pi/L\, x} \qquad c_n = \int_{-L}^{L} f(x) e^{-\frac{in\pi}{L}x}\, dx$$

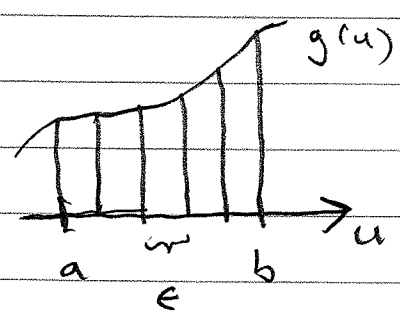
Here c_n will be $2L$ times bigger

compensated by dividing by $2L$ here.

Let's also introduce the notation $k = \frac{n\pi}{L}$

$$f(x) = \frac{1}{2L}\sum_{-\infty}^{\infty} c_k e^{ikx} \qquad c_k = \int_{-L}^{L} f(x) e^{-ikx}\, dx$$

Finally, recall the way we get integral as a Riemann sum ("rectangle rule")



$$\int_a^b g(u)\,du = \sum_n g_n \epsilon$$

ϵ spacing

values of g at discrete points

$$\sum_n g_n = \frac{1}{\epsilon}\int_a^b g(u)\,du$$

As $L \to \infty$ our k points get more and more closely spaced $\epsilon = \frac{\pi}{L}$. Converting to integral will become a good approximation

$$f(x) = \frac{1}{2L}\frac{L}{\pi}\int_{-\infty}^{\infty} c(k)\, e^{ikx}\, dk$$

$1/\epsilon$

choice of $\pm$ is arbitrary just must be opposite to each other

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} c(k)\, e^{ikx}\, dx \qquad c(k) = \int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, dx$$

This is called a "Fourier integral". These eqns look <u>very</u> similar to each other, emphasizing the $f(x)$ and $c(k)$ bases are really the same thing. Sometimes people even write

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} c(k)\, e^{ikx}\, dx \qquad c(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, dx$$

to make it look <u>really</u> identical.

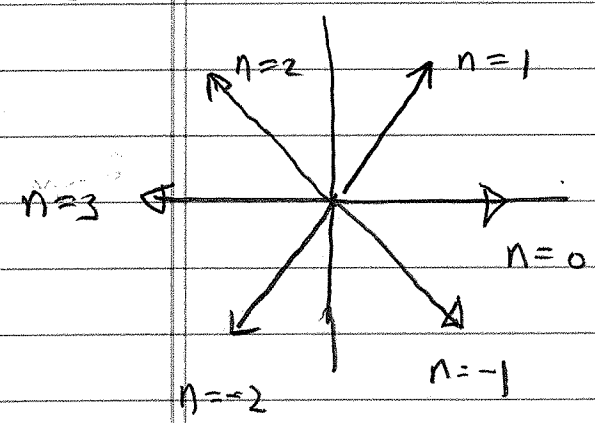
FI-5

Early in the course we noted that when

you sum up all the roots of 1 you get zero

$$\sum_{n=-\frac{L}{2}+1}^{L/2} e^{i\frac{2\pi}{L}n} = 0$$

$L=6$

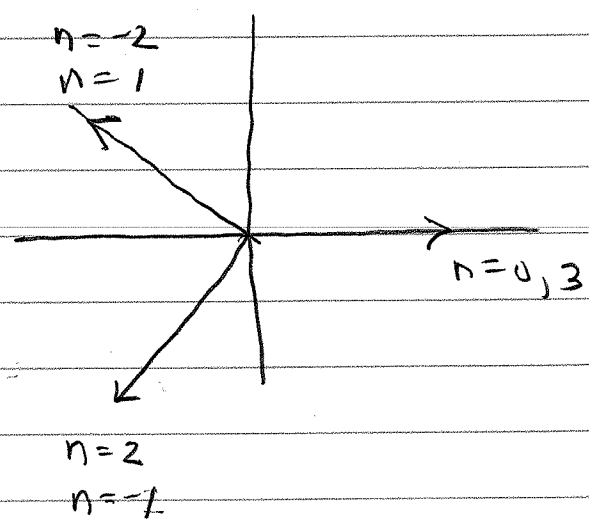


It is also true that

if you raise those roots to

the power p and add them

you get zero. eg for $p=2$:



unless, of course $p=0$ in which case the sum is L,

$$\sum_{n=-\frac{L}{2}+1}^{L/2} \left(e^{i\frac{2\pi}{L}n}\right)^p = L\,\delta_{p,0}$$

"Kronecker delta"

FI-6

If we define $k = \frac{2\pi n}{L}$ this tells us

$$\sum_k e^{ikp} = L\,\delta_{p,0}$$

and taking $L \to \infty$ and converting to integral as before

$$\frac{L}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ikp} = L\,\delta_{p,0}$$

$1/\epsilon$ factor

$$\int_{-\infty}^{\infty} dk\, e^{ikp} = 2\pi\,\delta_{p,0}$$

$$\int_{-\infty}^{\infty} dk\, e^{ikx} = 2\pi\,\delta(x)$$

FI-6A

Do FI-8-10 FIRST

The Fourier integral plays a particularly central role in QM. Real space wave function $\psi(x)$:

$$|\psi(x)|^2 dx = \text{prob of m particle has position between } x \text{ and } x+dx$$

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

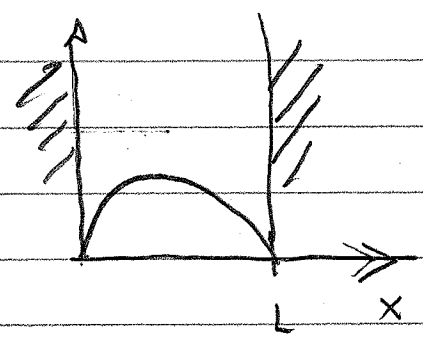
If $$\phi(p) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \psi(x)\, dx$$

$$|\phi(p)|^2 dp = \text{prob of m particle has momentum between } p \text{ and } p+dp$$

!!!

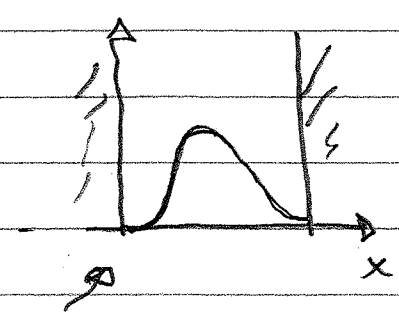
Consider $\psi(x) =$

$$= \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$$



prob $|\psi(x)|^2 = \frac{2}{L} \sin^2 \frac{\pi x}{L}$

sort of same shape



Q: why?

A: $\sin x \sim x$

$\sin^2 x \sim x^2$

FJ-6B

Q: What is probability particle has momentum p?!

Any guesses?

$$\phi(p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \sqrt{\frac{2}{L}} \sin\frac{\pi x}{L}\, e^{-ipx/\hbar}\, dx$$

$$= \frac{1}{\sqrt{2\pi}} \int_0^L \sqrt{\frac{2}{L}}\, \frac{e^{i\pi x/L} - e^{-i\pi x/L}}{2}\, e^{ipx/\hbar}\, dx$$

$$= \frac{1}{\sqrt{2\pi}}\, \frac{1}{2}\sqrt{\frac{2}{L}} \int_0^L \left(e^{i(\pi/L + p/\hbar)x} - e^{i(-\pi/L + p/\hbar)x} \right) dx$$

$$\frac{e^{i(\pi/L + p/\hbar)x}}{i(\pi/L + p/\hbar)} \Bigg|_0^L -$$

$$\frac{-e^{ipL/\hbar} - 1}{i(\pi/L + p/\hbar)} \pm \frac{-e^{ipL/\hbar} - 1}{i(-\pi/L + p/\hbar)}$$

$$= \frac{1 + e^{ipL/\hbar}}{i} \left\{ \frac{+\pi/L - p/\hbar + \pi/L + p/\hbar}{(\pi/L + p/\hbar)(-\pi/L + p/\hbar)} \right\}$$

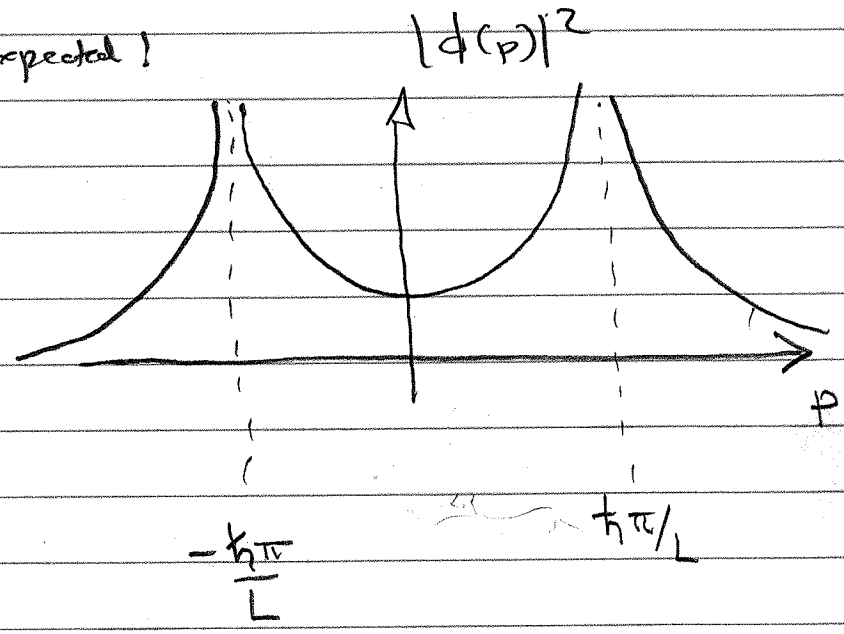
$$= \frac{2\pi}{iL} \left(1 + e^{ipL/\hbar}\right) \frac{1}{p^2/\hbar^2 - \pi^2/L^2}$$

FI-6C

$$|\phi(p)|^2 = \frac{2\pi}{L}\left(\frac{p^2}{\hbar^2} - \frac{\pi^2}{L^2}\right)^{-2} \underbrace{(1+e^{ipL/\hbar})(1-e^{-ipL/\hbar})}_{2(1+\cos pL/\hbar)}$$

peaked at $p = \pm \hbar\pi/L$

as expected!



check normalization!

FOURIER

SERIES

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{inx\pi/L}$$

$$c_n = \frac{1}{2L}\int_{-L}^{L} f(x)\, e^{-inx\pi/L}\, dx$$

$$\int_{-L}^{L} e^{+inx\pi/L} e^{-imx\pi/L}\, dx = 2L\delta_{n,m}$$

Kronecker delta

INTEGRAL

$$f(x) = \frac{1}{\sqrt{2\pi}}\int dk\, c(k)\, e^{ikx}$$

$$c(k) = \frac{1}{\sqrt{2\pi}}\int dx\, f(x)\, e^{-ikx}$$

$$\int_{-\infty}^{\infty} e^{+ikx} e^{-ik'x} = 2\pi\delta(k-k')$$

Diracdelta function

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{inx\pi/L}$$

$$e^{-imx\pi/L} f(x) = \sum_{n=-\infty}^{\infty} c_n e^{inx\pi/L} e^{-imx\pi/L}$$

$$\downarrow$$

$$2L\delta_{nm}$$

Then $\int_{-L}^{L} dx$

$$\int_{-L}^{L} e^{-imx\pi/L} f(x)\, dx = 2L\, c_m$$

$$e^{-ik'x} f(x) = \frac{1}{\sqrt{2\pi}}\int dk\, c(k)\, e^{-ik'x} e^{ikx}$$

integrate dx

$$\int_{-\infty}^{\infty} dx\, f(x)\, e^{-ik'x} = \frac{1}{\sqrt{2\pi}}\, 2\pi\, c(k')$$

Applications of Fourier Integrals - II

① QM $\psi(x,0) = n e^{-x^2/2\Delta^2}$ ← start with wave function which is gaussian of width Δ

normalization

$$\int_{-\infty}^{\infty} |\psi(x,0)|^2 dx = n^2 \int_{-\infty}^{\infty} e^{-x^2/\Delta^2} dx = n^2 \sqrt{\pi\Delta^2} = n^2\sqrt{\pi}\Delta$$

Thus $n = \frac{1}{\sqrt{\Delta}} \frac{1}{\pi^{1/4}}$

Dimensions: Δ has units of Length and ψ of $1/\sqrt{L}$ W

Free particle $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x,t) = -\frac{\hbar}{i}\frac{\partial\psi(x,t)}{\partial t}$

$$\psi(x,t) = f(x)g(t)$$

$$\frac{-\frac{\hbar^2}{2m} d^2f/dx^2}{f(x)} = \frac{-\frac{\hbar}{i}\, dg/dt}{g} = E$$

$$\frac{d^2f}{dx^2} = \frac{-2mE}{\hbar^2} f(x) \qquad \frac{dg}{dt} = \frac{-iE}{\hbar} g$$

Define $E = \hbar^2 k^2/2m$ $\qquad g(t) = e^{-iEt/\hbar}$

$$\frac{d^2f}{dx^2} = -k^2 f$$

$f(x) = e^{ikx}$ ← Used sine, cosine in a box but complex exponential (plane wave) simpler here.

FI-8

$$\psi(x,t) = \int_{-\infty}^{\infty} c(k)\, e^{ikx}\, \underbrace{e^{-i/\hbar\, \hbar^2 k^2/2m\, t}}_{\text{soln for single } k}\, dk$$

linear combination

$$\int_{-\infty}^{\infty} e^{-ax^2}\, dx = \sqrt{\frac{\pi}{a}}$$

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2}\, dx = \frac{1}{2a}\sqrt{\frac{\pi}{a}}$$

$$n = 1/\Delta\sqrt{\pi}$$

$$\psi(x,0) = n\, e^{-x^2/2\Delta^2} = \int_{-\infty}^{\infty} c(k)\, e^{ikx}\, dk$$

$$\int_{-\infty}^{\infty} d\vec{x}\, e^{-x^T A x} = \frac{\pi^{N/2}}{\sqrt{\det A}}$$

$N = \dim A$

$$\int_{-\infty}^{\infty} x_i x_j\, d\vec{x}\, e^{-x^T A x} = \frac{1}{2} (A^{-1})_{ij} \frac{\pi^{N/2}}{\sqrt{\det A}}$$

$$c(k) = \frac{1}{\sqrt{2\pi}}\, n \int_{-\infty}^{\infty} e^{-x^2/2\Delta^2}\, e^{-ikx}\, dx$$

complete the square

$$-\frac{x^2}{2\Delta^2} - ikx = -\frac{1}{2\Delta^2}\left(x^2 + 2ik\Delta^2 x\right)$$

$$= -\frac{1}{2\Delta^2}\left(x + ik\Delta^2\right)^2 + \frac{1}{2\Delta^2}\left(ik\Delta^2\right)^2$$

$$= -\frac{1}{2\Delta^2}\left(x + ik\Delta^2\right)^2 - \frac{k^2\Delta^2}{2}$$

Wicks Theorem... Quantum Field Theory

Amazingly.. true even if

$$\int_{-\infty}^{\infty} e^{-a(x-x_0)^2}\, dx = \sqrt{\frac{\pi}{a}}$$

x_0 real or complex

$$c(k) = \frac{1}{\sqrt{2\pi}}\, n\, e^{-k^2\Delta^2/2} \underbrace{\int_{-\infty}^{\infty} e^{-1/2\Delta^2 (x + ik\Delta^2)^2}\, dx}_{\text{still } \sqrt{2\pi\Delta^2}}$$

still $\sqrt{2\pi\Delta^2}$ even though $ik\Delta^2$ is in argument of exponential

$$c(k) = \frac{n\Delta}{\sqrt{2\pi}}\, e^{-k^2\Delta^2/2}$$

FI-9

Recall $c(k)$ are coefficients of $\vec{\psi}$ in the new "Fourier basis". We can check normalization

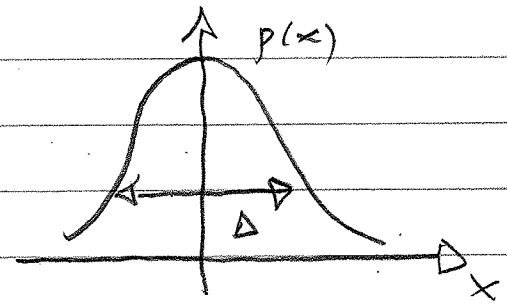
$$\int_{-\infty}^{\infty} |c(k)|^2 dk = \frac{n^2 \Delta^2}{2\pi} \sqrt{\frac{2\pi}{\Delta^2}}$$

$$n^2 = \frac{1}{\Delta\sqrt{\pi}} \qquad = \frac{1}{\Delta}\frac{1}{\sqrt{\pi}}\frac{\Delta^2}{2\pi}\frac{\sqrt{2\pi}}{\Delta} = 1$$

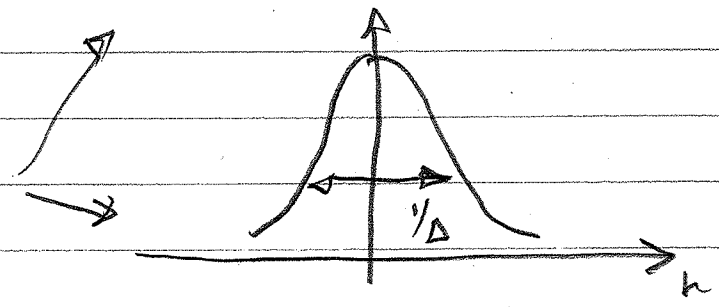
Just as $p(x) = |\psi(x)|^2$ is probability to find particle at location x

$\tilde{p}(k) = |c(k)|^2$ is probability to find particle with momentum $\hbar k$

$p(x) \sim e^{-x^2/\Delta^2}$



$\tilde{p}(k) \sim e^{-k^2\Delta^2}$



Q: What does this remind you of

FI-10

Uncertainty principle!

If $p(x)$ is made narrow by making Δ small

$\tilde{p}(k)$ gets wide $(1/\Delta)$

cannot know both x and k to arbitrary accuracy simultaneously.

$$\left\{\begin{matrix}\text{width of}\\ x\end{matrix}\right\}\left\{\begin{matrix}\text{width}\\ \text{of } k\end{matrix}\right\} \sim 1$$

$$\uparrow$$

$$\left\{\begin{matrix}\text{width of}\\ x\end{matrix}\right\}\left\{\begin{matrix}\text{width of}\\ p\end{matrix}\right\} \sim \hbar \qquad !!$$

$$p = \hbar k$$

Uncertainty principle $\longleftrightarrow$ Fourier integral.

It is quite messy algebraically to get $\psi(x,t)$

$$\psi(x,t) = \int dk\, c(k)\, e^{-i/\hbar\, \hbar^2 k^2/2m\, t}\, e^{ikx}$$

$$\uparrow$$

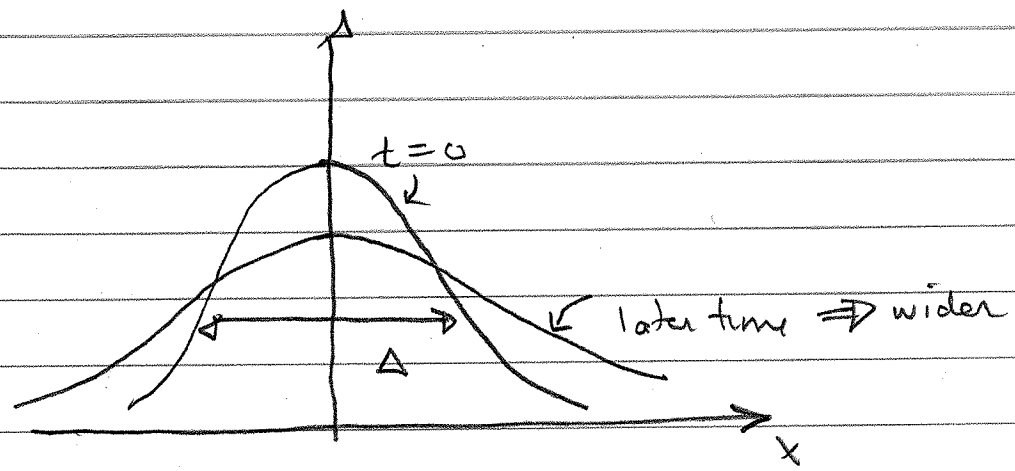
$$\frac{n\Delta}{\sqrt{2\pi}}\, e^{-k^2\Delta^2/2}$$

Complete square etc.

Q Can anyone guess what happens?

width of wave packet spreads with time,

stays centered at origin



An interesting calculation

$$\psi(x,0) = n\, e^{-x^2/2\Delta^2}\, e^{ik_0 x}$$

Q: What happens?

A: Wave function moves and spreads

FI-12

$n^2 = 1/\Delta\sqrt{\pi}$

Uncertainty principle

$\psi(x) = n\, e^{-x^2/2\Delta^2}$ $\qquad$ $c(k) = n\Delta\, e^{-k^2\Delta^2/2}$

$\Delta x^2 = \langle x^2\rangle - \langle x\rangle^2$ $\qquad$ $\Delta p^2 = \langle p^2\rangle - \langle p\rangle^2$

ϕ by symmetry

$$\langle x^2\rangle = \int_{-\infty}^{\infty} x^2 |\psi(x)|^2 dx = \int_{-\infty}^{\infty} x^2 n^2 e^{-x^2/2\Delta^2} dx$$

$$= n^2 \sqrt{\pi\Delta^2}\, \frac{\Delta^2}{2} = \frac{1}{\Delta\sqrt{\pi}} \sqrt{\pi\Delta^2}\, \frac{\Delta^2}{2} = \frac{\Delta^2}{2}$$

$$\langle p^2\rangle = \int_{-\infty}^{\infty} |c(k)|^2 (\hbar k)^2 dk$$

$$= \hbar^2 \int_{-\infty}^{\infty} n^2\Delta^2 k^2 e^{-k^2\Delta^2} dk$$

$$= n^2\Delta^2\hbar^2 \sqrt{\frac{\pi}{\Delta^2}}\, \frac{1}{2\Delta^2} = \frac{1}{\Delta\sqrt{\pi}} \Delta^2 \hbar^2 \sqrt{\frac{\pi}{\Delta^2}}\, \frac{1}{2\Delta^2}$$

$$= \hbar^2/2\Delta^2$$

$$\Delta x \Delta p = \frac{\Delta}{\sqrt{2}} \frac{\hbar}{\sqrt{2}\Delta} = \frac{\hbar}{2}$$ $\longleftarrow$ smallest possible value!

Solving the Diffusion Eqn

$$\frac{\partial \phi(x,t)}{\partial t} = D \frac{\partial^2 \phi(x,t)}{\partial x^2}$$

AKA imaginary time Schroedinger Eqn : $i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\psi(x,t)$

$$\phi(x,t) = f(x)\,g(t)$$

$$f(x)\,g'(t) = D\,f''(x)\,g(t)$$

$$\frac{f''(x)}{f(x)} = \frac{1}{D}\frac{g'(t)}{g(t)} = -k^2$$

$$f(x) = e^{ikx} \qquad g(t) = e^{-Dk^2 t}$$

$$\phi(x,t) = \int dk\, c(k)\, e^{ikx} e^{-Dk^2 t}$$

$$\phi(x,0) = \int dk\, c(k)\, e^{ikx}$$

$$c(k) = \int \frac{dx}{2\pi}\, \phi(x,0)\, e^{-ikx}$$

Eg $\phi(x,0) = \delta(x) \qquad c(k) = \frac{1}{2\pi}$

(Like schroedinger Eqn / uncertainty
perfectly localized in real space
completely spread out in K space)

$$\phi(x,t) = \int dk \, \frac{1}{2\pi} e^{ikx} e^{-Dk^2 t}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \; e^{-Dt(k^2 - ix/Dt2)^2} e^{+Dt(ix/2Dt)^2}$$

$$= \frac{1}{2\pi} \sqrt{\frac{\pi}{Dt}} \; e^{-x^2/4Dt}$$

$$= \frac{1}{\sqrt{4\pi Dt}} \; e^{-x^2/4Dt}$$

Normalization $\int_{-\infty}^{\infty} \phi(x,t)\,dx = \frac{1}{\sqrt{4\pi Dt}} \sqrt{\frac{\pi}{1/4Dt}} = 1$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 \, \phi(x,t)\,dx = \frac{1}{\sqrt{4\pi Dt}} \frac{1}{2\frac{1}{4Dt}} \sqrt{4\pi Dt}$$

$$\langle x^2 \rangle = 2Dt$$

$$\sqrt{\langle x^2 \rangle} \sim t^{1/2}$$ <u>Diffusion</u>