"Free Particle" evolution in x and t

Time-dependent Schrödinger Eqn, $V(x)=0$: $$i\hbar \frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi$$

$$\Longrightarrow \quad \frac{\partial \psi}{\partial t} = \left(\frac{\hbar i}{2m}\right)\frac{\partial^2}{\partial x^2}\psi$$

This looks just like the classical diffusion eqn. but with <u>imaginary</u> coef. $D \to iD = i\hbar/2m$!

So we know how to solve it, via separation of variables

or just substitution of the Fourier form $\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\tilde{\psi}(k,t)\,e^{ikx}dk$.

The result (see lec. 3) is $\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} A(k)\,e^{-(iD)k^2 t}\,e^{ikx}\,dk$, where $A(k)$

is the Fourier transform of initial conditions $\psi(x,t=0)$.

<u>Example Initial conditions</u> : normalized gaussian $\psi(x,t=0) = \left(\frac{2a}{\pi}\right)^{1/4} e^{-ax^2}$ $\left(\text{note: } \int_{-\infty}^{\infty}\psi^*\psi\,dx = 1\right)$

Probability density $\psi^*\psi$ has a width $\Delta x = \frac{1}{2\sqrt{a}}$.

The Fourier transform (again, see lec. 3) is $A(k) = \frac{1}{(2a\pi)^{1/4}}\,e^{-\frac{k^2}{4a}}$.

Calculation of $\psi(x,t)$

Substitute $A(k)$:

$$= \left(\frac{1}{2\pi}\right)^{3/4} \frac{1}{a^{1/4}} \int_{-\infty}^{\infty} e^{-\frac{k^2}{4a}} \, e^{-iDk^2 t} \, e^{ikx} \, dk$$

Factor exponent:

$$= \left(\frac{1}{2\pi}\right)^{3/4} \frac{1}{a^{1/4}} \int_{-\infty}^{\infty} e^{-\left(\frac{1}{4a} + iDt\right)\left(k^2 - \frac{ikx}{\frac{1}{4a} + iDt}\right)} dk$$

Complete the square:

$$= \left(\frac{1}{2\pi}\right)^{3/4} \frac{1}{a^{1/4}} \int_{-\infty}^{\infty} e^{-\left(\frac{1}{4a} + iDt\right)\left(k - \frac{ix}{2\left(\frac{1}{4a} + iDt\right)}\right)^2} e^{-\frac{x^2}{4\left(\frac{1}{4a} + iDt\right)}} dk$$

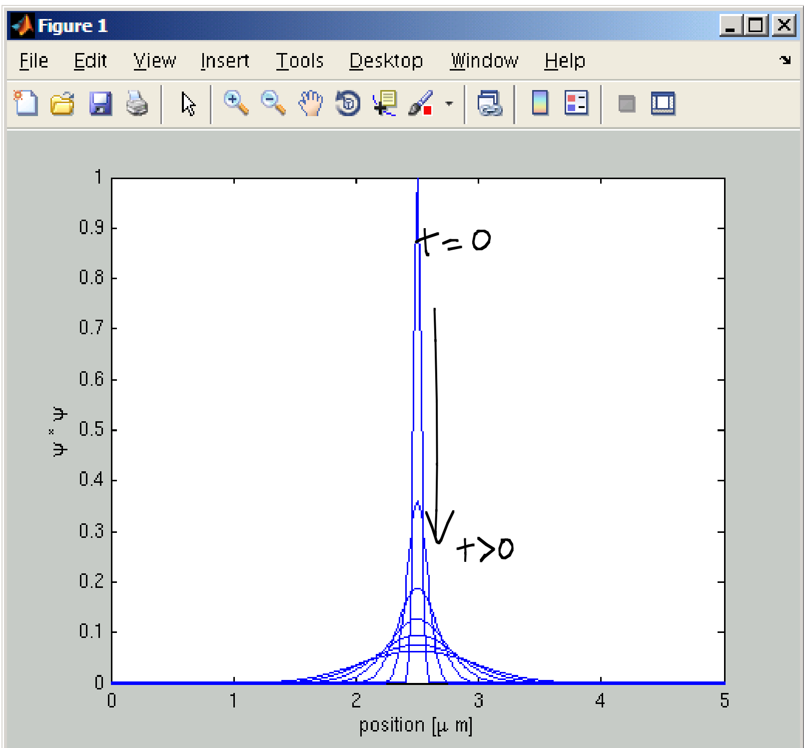
Perform definite integral over gaussian:

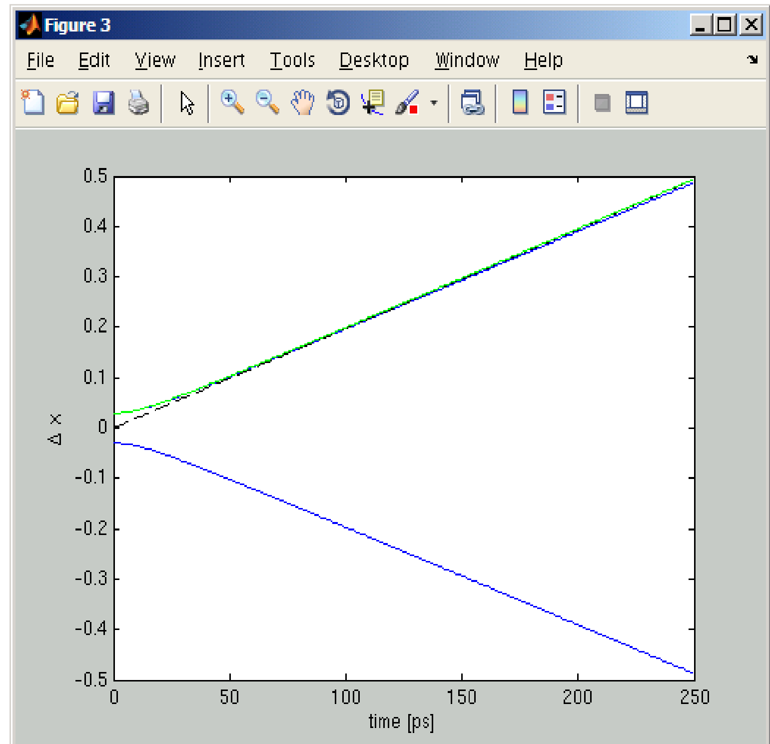
$$= \left(\frac{1}{2\pi}\right)^{3/4} \frac{1}{a^{1/4}} \sqrt{\frac{\pi \, 4a}{1 + 4iDat}} \, e^{-\frac{ax^2}{1+4iDat}} = \left(\frac{2a}{\pi}\right)^{1/4} \frac{1}{\sqrt{1+4iDat}} \, e^{\frac{-ax^2}{1+4iDat}}$$

Don't panic about a complex gaussian! Only $\psi^* \psi$ is physically meaningful!

Probability density evolution

$$\psi^*\psi \propto e^{-\frac{ax^2}{1-4iDat}}\, e^{-\frac{ax^2}{1+4iDat}} = e^{-2ax^2\left(\frac{1}{1+16D^2a^2t^2}\right)} = e^{-\frac{x^2}{2\Delta x^2}}$$ where $\Delta x = \sqrt{\frac{1+16D^2a^2t^2}{4a}}$, $D = \frac{\hbar}{2m}$



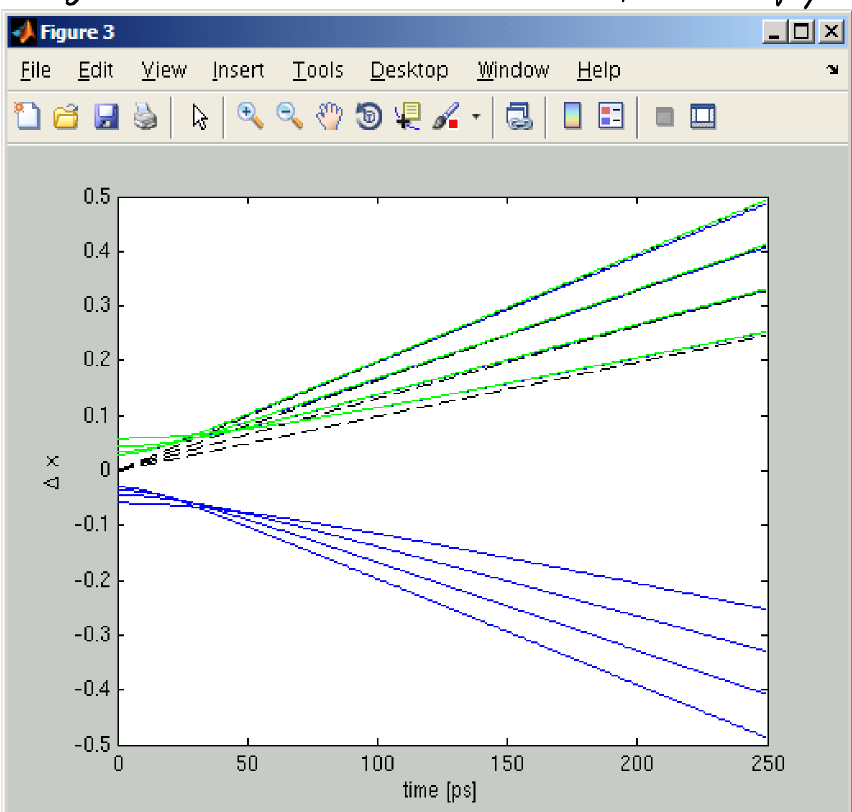


Just like the classical diffusion equation, the distribution widens and the maximum decreases to conserve the total probability $\int_{-\infty}^{\infty} \psi^*\psi\, dx = 1$

C.f. Sol'n to classical equation of motion for $V(x)=0$, and I.C.s $x(t=0)=0$, $\dot{x}(t=0)=0$!

Heisenberg uncertainty principle

Note that for large t when $D^2a^2t^2 \gg 1$, $\Delta x \approx 2D\sqrt{a}\,t$.
This means that the gaussian grows Faster for more localized initial conditions (Δx small / $\sqrt{a}$ large). This is the "Heisenberg" uncertainty principle $\Delta x \Delta p \geq \hbar/2$ at work: small Δx gives large momentum uncertainty Δp, which causes faster broadening!



An analogy:

This looks like an optical beam emerging from a focal point along its propagation axis!

$\Rightarrow$ The uncertainty principle is also the reason why you should use the shortest focal distance lens w/ the largest aperture diameter to get the smallest focal point and highest optical resolution! (microscopes / telescopes)

Derivation of Optical Schrödinger Equation

Classical wave equation governing E+M wave propagation:

$$\nabla^2 \vec{\mathcal{E}} = \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\vec{\mathcal{E}}$$

Assume the beam is cylindrically-symmetric about propagation direction $\hat{z}$ and polarized along $\hat{x}$:

$$\vec{\mathcal{E}} = \mathcal{E}_x(x,z)\, e^{i(kz-\omega t)}\,\hat{x}$$

Then,

$$\frac{\partial^2 \mathcal{E}_x}{\partial x^2} e^{i(kz-\omega t)} + \frac{\partial^2}{\partial z^2}\left(\mathcal{E}_x e^{i(kz-\omega t)}\right) = \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\mathcal{E}_x e^{i(kz-\omega t)}$$

Distributing the derivative and cancelling common terms yields:

$$\frac{\partial^2 \mathcal{E}_x}{\partial x^2} e^{i(kz-\omega t)} + \frac{\partial}{\partial z}\left(\frac{\partial \mathcal{E}_x}{\partial z} e^{i(kz-\omega t)} + ik\,\mathcal{E}_x e^{i(kz-\omega t)}\right) = \frac{-\omega^2}{c^2}\mathcal{E}_x e^{i(kz-\omega t)}$$

$$\frac{\partial^2 \mathcal{E}_x}{\partial x^2} \cancel{e^{i(kz-\omega t)}} + \frac{\partial^2}{\partial z^2}\mathcal{E}_x \cancel{e^{i(kz-\omega t)}} + ik\frac{\partial \mathcal{E}_x}{\partial z}\cancel{e^{i(kz-\omega t)}} + ik\left(\frac{\partial}{\partial z}\mathcal{E}_x \cancel{e^{i(kz-\omega t)}} + ik\,\mathcal{E}_x \cancel{e^{i(kz-\omega t)}}\right) = \frac{-\omega^2}{c^2}\mathcal{E}_x \cancel{e^{i(kz-\omega t)}}$$

$$\frac{\partial^2 \mathcal{E}_x}{\partial x^2} + \frac{\partial^2}{\partial z^2}\mathcal{E}_x + 2ik\frac{\partial \mathcal{E}_x}{\partial z} - k^2\mathcal{E}_x = \frac{-\omega^2}{c^2}\mathcal{E}_x$$

Slowly-varying envelope approximation

Now, we know that $\omega = kc$ (classical wave dispersion), so:

$$\frac{\partial^2 \mathcal{E}_x}{\partial x^2} + \frac{\partial^2}{\partial z^2}\mathcal{E}_x + 2ik\frac{\partial \mathcal{E}_x}{\partial z} = 0$$

Notice that if we ignore $\frac{\partial^2}{\partial z^2}\mathcal{E}_x$ ("slowly varying envelope approx"), we have

$$\frac{\partial^2 \mathcal{E}_x}{\partial x^2} = (-2k)i\frac{\partial \mathcal{E}_x}{\partial z}$$

This is mathematically the same as our Schrödinger equation

$$\frac{\partial^2 \psi}{\partial x^2} = \left(\frac{2m}{\hbar}\right)i\frac{\partial \psi}{\partial t}$$

but w/different coef. and $t \to z$! So if the beam has a gaussian intensity cross-section, we can expect it to diffract along propagation direction in approx. same way as QM probability evolves in time!