One Dimensional Problems

4-1

Free - Particle Motion

We begin our discussion of the solution to Schroedinger's equation with the free particle problem:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t).$$

We can perform the usual separation of variables by writing

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

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2}{dx^2}\psi(x) = i\hbar\frac{1}{f(t)}\frac{d}{dt}f(t)$$

Equating each side to the energy E, we have

i) for the time dependence: $i\hbar\frac{1}{f(t)}\frac{d}{dt}f(t) = E$

$$\frac{d}{dt}f(t) = \frac{E}{i\hbar}f(t)$$

$$\text{or } f(t) = \underbrace{N}_{\text{normalization constant}} e^{-\frac{iEt}{\hbar}}.$$

ii) for the spatial dependence:

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2}{dx^2}\psi(x) = E = \frac{p^2}{2m}$$

(where p is <u>not</u> an operator)

$$\frac{d^2}{dx^2}\psi(x) = -\left(\frac{p}{\hbar}\right)^2\psi(x)$$

So we have two solutions. We can find out which one corresponds to what motion by taking

$$\hat{p}_x \psi_{\pm}(x) = -i\hbar \frac{d}{dx}\left(N' e^{\pm \frac{ipx}{\hbar}}\right)$$

$$= -i\hbar N' \left(\pm i \frac{p}{\hbar}\right) e^{\pm \frac{ipx}{\hbar}}$$

$$= \pm p \left[N' e^{\pm \frac{ipx}{\hbar}}\right]$$

$\Rightarrow$ ψ_+ travels to the right ; ψ_- travels to the left.

This solution has a few problems. First, it isn't localized:

$$\int \psi^* \hat{x}^2 \psi \, dx = N'^2 \int e^{-\frac{ipx}{\hbar}} x^2 e^{+\frac{ipx}{\hbar}} dx$$

(Don't do $\int \psi x \psi dx$ since it vanishes by symmetry)

$$= N'^2 \int_{-\infty}^{\infty} x^2 dx$$

diverges!

Second, N itself involves a divergent quantity.

$$1 = N'^2 \int_{-\infty}^{\infty} e^{-\frac{ipx}{\hbar}} e^{+\frac{ipx}{\hbar}} dx = N'^2 \int_{-\infty}^{\infty} dx .$$

The problem, of course, is that we have specified p exactly, so we have lost all information about x. To do better, we must construct a <u>wave packet</u> which includes a finite uncertainty in x, p.

- Box normalization:

$$1 = N^2 \int_{-L}^{L} e^{-ipx/\hbar} e^{+ipx/\hbar} dx = N^2 (2L) \; . \Rightarrow N^2 = \frac{1}{2L} \; .$$

$$\langle x^2 \rangle = N^2 \int_{-L}^{L} e^{-ipx/\hbar} x^2 e^{ipx/\hbar} dx = N^2 \cdot \frac{2}{3}(L)^3 = \frac{1}{2L} \frac{2}{3} L^3$$

$$= \frac{L^2}{3} \; .$$

$\therefore \langle x^2 \rangle$ diverges, even though $N^2 \to 0$.

Since $\bar{x} = 0$, then $\Delta x^2 = \langle x^2 \rangle$.

What about Δp^2?

$$\Delta p^2 = \int_{-L}^{L} \psi^* (\hat{p} - \bar{p})^2 \psi \, dx$$

$$= \frac{1}{2L} \int_{-L}^{L} e^{-ipx} \underline{\underline{(\bar{p} - \bar{p})}}^2 e^{ipx} dx$$

How fast does this go to zero?
Take limit of Gaussian?
Does it make any difference that
$P = n \frac{\hbar}{2L}$ (quantization within box)?
$n = 1, 2, 3 \cdots$

Wave Packets [Schiff, pg. 60-63].

We need some definitions:

$$\langle \hat{x} \rangle \equiv \bar{x}$$
$$\langle \hat{p} \rangle \equiv \bar{p}$$
$$\hat{\alpha} = \hat{x} - \bar{x}$$
$$\hat{\beta} = \hat{p} - \bar{p}$$

Let's go back to Heisenberg's uncertainty relation for a moment.

$$\Delta x^2 = \int \psi^* \hat{\alpha}^2 \psi \, dx \quad \& \quad \Delta p^2 = \int \psi^* \hat{\beta}^2 \psi \, dx$$

$$\Rightarrow \Delta x^2 \cdot \Delta p^2 = \int (\underbrace{\hat{\alpha}\psi}_{f})^* (\alpha\psi) \, dx \cdot \int (\underbrace{\hat{\beta}\psi}_{g})^* (\beta\psi) \, dx$$

The way we get to the uncertainty principle is via

$$\int |f|^2 dx \cdot \int |g|^2 dx \geq \left| \int f^* g \right|^2$$

[Analogue to $\left(\sum_i f_i^2\right) \cdot \left(\sum_i g_i^2\right) \geq \left(\sum_i f_i g_i\right)^2$]

The equality holds only if $f = \gamma g$ (γ constant).

or

$$\hat{\alpha}\psi = \gamma \hat{\beta} \psi \quad (1).$$

Going through the uncertainty proof again,

$$\Delta x^2 \cdot \Delta p^2 \geq \left| \int \psi^* \hat{\alpha} \hat{\beta} \psi \, dx \right|^2.$$

Let's work on the r.h.s. a little more:

rewrite

$$\alpha\beta = \frac{1}{2}\left[\hat{\alpha}\hat{\beta} - \hat{\beta}\hat{\alpha}\right] + \frac{1}{2}\left[\hat{\alpha}\hat{\beta} + \hat{\beta}\hat{\alpha}\right]$$

$$\Rightarrow \Delta x^2 \cdot \Delta p^2 \geq \frac{1}{4}\left| \int \psi^* (\hat{\alpha}\hat{\beta} - \hat{\beta}\hat{\alpha})\psi \, dx \right|^2 + \frac{1}{4}\left| \int \psi^* (\hat{\alpha}\hat{\beta} + \hat{\beta}\hat{\alpha})\psi \, dx \right|^2 .$$

+ cross terms which vanish.

Now, the first term becomes:

$$\begin{aligned}
\hat{\alpha}\hat{\beta} - \hat{\beta}\hat{\alpha} &= (\hat{x} - \bar{x})(\hat{p} - \bar{p}) - (\hat{p} - \bar{p})(\hat{x} - \bar{x}) \\
&= \hat{x}\hat{p} - \hat{x}\bar{p} - \bar{x}\hat{p} + \bar{x}\bar{p} - (\hat{p}\hat{x} - \hat{p}\bar{x} - \bar{p}\hat{x} + \bar{x}\bar{p}) \\
&= \hat{x}\hat{p} - \hat{p}\hat{x} \\
&= i\hbar \hat{1} .
\end{aligned}$$

$$\Rightarrow \Delta x^2 \cdot \Delta p^2 \geq \frac{1}{4}\hbar^2 + \underbrace{\frac{1}{4}\left| \int \psi^* (\hat{\alpha}\hat{\beta} + \hat{\beta}\hat{\alpha})\psi \, dx \right|^2}_{\text{must also vanish.}}$$

So the conditions on the minimum wavepacket are

$$\hat{\alpha}\psi = \gamma\hat{\beta}\psi \qquad (1)$$

$$\int \psi^* (\hat{\alpha}\hat{\beta} + \hat{\beta}\hat{\alpha})\psi \, dx = 0 \qquad (2)$$

Let's look at (1):

$$(\hat{x} - \bar{x})\psi = \gamma(\hat{p} - \bar{p})\psi$$

$$\Rightarrow \hat{p}\psi = \bar{p}\psi + \frac{1}{\gamma}(\hat{x} - \bar{x})\psi .$$

Substituting $\hat{p} = -i\hbar\frac{d}{dx}$; $\hat{x}\psi = x\psi$

or $\frac{d}{dx}\psi = \frac{i\bar{p}}{\hbar}\psi + \frac{i}{\gamma\hbar}(x-\bar{x})\psi$

This is really a differential equation for $\psi(x)$. The solution is:

$$\psi(x) = \underset{\substack{\uparrow \\ \text{normalization} \\ \text{constant}}}{N} \exp i\left[\frac{1}{2\gamma\hbar}(x-\bar{x})^2 + \frac{\bar{p}x}{\hbar}\right].$$

Proof:

$$\frac{d}{dx}\psi = N\frac{d}{dx}e^{i\left[\frac{1}{2\gamma\hbar}(x-\bar{x})^2 + \frac{\bar{p}x}{\hbar}\right]}$$

$$= N\left(i\frac{1}{2\gamma\hbar}2(x-\bar{x}) + i\frac{\bar{p}}{\hbar}\right)e^{i\left[\frac{1}{2\gamma\hbar}(x-\bar{x})^2 + \frac{\bar{p}x}{\hbar}\right]}.$$

$$= i\left(\frac{1}{\gamma\hbar}(x-\bar{x}) + \frac{\bar{p}}{\hbar}\right)\psi.$$

This is an amusing result. We have $\psi = N \cdot \text{gaussian} \times e^{i\bar{p}x/\hbar}$. Looks like Schrodinger's equation result, without using S.E. Note, however, that we have

1. gaussian in x.
2. $e^{i\bar{p}x/\hbar}$ involves $\bar{p}$, not p.

We are left with two constants to evaluate, N & γ.

Solution for N, γ.

We start by finding a property of γ.

From condition #2 $\qquad \hat{\beta} = \frac{\hat{\alpha}}{\gamma} \qquad \overleftarrow{\hat{\beta}} = \frac{\overleftarrow{\hat{\alpha}}}{\gamma^*}$

$$\int \psi^* (\hat{\alpha}\hat{\beta} + \hat{\beta}\hat{\alpha}) \psi \, dx = 0 \Rightarrow \int \psi^* \left(\frac{1}{\gamma} \hat{\alpha}^2 + \frac{1}{\gamma^*} \hat{\alpha}^2 \right) \psi \, dx$$
$$= \left(\frac{1}{\gamma} + \frac{1}{\gamma^*} \right) \int \psi^* \hat{\alpha}^2 \psi \, dx$$
$$= 0 \text{ only if } \gamma \text{ is pure imaginary.}$$

To solve for N and subsequently γ, we use the normalization condition:

$$1 = \int \psi^* \psi \, dx = N^2 \int \exp\left[\frac{-i}{2\gamma^* \hbar} (x - \bar{x})^2 - \frac{i\bar{p}x}{\hbar} \right] \times$$
$$\exp\left[\frac{i}{2\gamma\hbar} (x - \bar{x})^2 + \frac{i\bar{p}x}{\hbar} \right] dx$$
$$= N^2 \int \exp\left(i \left(\frac{1}{\gamma} - \frac{1}{\gamma^*} \right) \frac{(x-\bar{x})^2}{2\hbar} \right) dx$$

For this to converge, γ must be negative imaginary:

$$\gamma = -i\xi \qquad \text{with } \xi > 0 \text{ ; real.}$$

$$\Rightarrow \quad i\left(\frac{1}{\gamma} - \frac{1}{\gamma^*} \right) = i\left(\frac{-1}{i\xi} - \left(\frac{1}{i\xi} \right) \right) = -\frac{2}{\xi} .$$

$$\Rightarrow \quad 1 = N^2 \int \exp\left(-\frac{1}{\xi\hbar} (x - \bar{x})^2 \right) dx = N^2 \int \exp\left(-\frac{1}{\xi\hbar} y^2 \right) dy$$
$$= N^2 \sqrt{\xi\hbar} \int_{-\infty}^{\infty} \exp(-z^2) \, dz$$
$$= N^2 \sqrt{\xi\hbar} \cdot 2 \cdot \frac{\sqrt{\pi}}{2} = N^2 \sqrt{\pi\xi\hbar}$$

Proofs of Integrals.

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1. $I = \int_{-\infty}^{\infty} e^{-x^2}\, dy$

$$I^2 = \int_{-\infty}^{\infty} e^{-x^2}\, dx \int_{-\infty}^{\infty} e^{-y^2}\, dy$$
$$= \iint e^{-(x^2+y^2)}\, dx\, dy$$

Change to polar coords: $x^2+y^2 = r^2$
$dx\, dy = r\, dr\, d\theta$

$$I^2 = \int_0^{2\pi} d\theta \int_0^{\infty} e^{-r^2}\, r\, dr.$$

Then substitute $\xi = e^{-r^2}$ $\quad \frac{d\xi}{dr} = -2r e^{-r^2}$

$$\Rightarrow I^2 = 2\pi \int_1^0 \left(-\tfrac{1}{2}\right) d\xi$$
$$= -\pi\, \xi\Big|_1^0 = \pi.$$

$\therefore I = \sqrt{\pi}$

2. $\int z^2 e^{-z^2}\, dz$

Parametric from
$$I(n) = \int_0^{\infty} e^{-\alpha x^2} x^n\, dx$$
$$I(n) = -\frac{\partial}{\partial \alpha}\left(\int_0^{\infty} e^{-\alpha x^2} x^{n-2}\, dx \right).$$
$$I(2) = -\frac{\partial I(0)}{\partial \alpha} = -\frac{\sqrt{\pi}}{2} \frac{\partial}{\partial \alpha}\left(\alpha^{-1/2}\right)$$
$$= \frac{\sqrt{\pi}}{4}\, \alpha^{-3/2}$$

or, $N = \dfrac{1}{\sqrt[4]{\pi \xi \hbar}}$

Lastly, we solve for ξ in terms of Δx:

$$(\Delta x)^2 = \int (x-\bar{x})^2 \, |\psi|^2 \, dx$$

$$= N^2 \int (x-\bar{x})^2 \, e^{-\frac{1}{\xi\hbar}(x-\bar{x})^2} \, dx$$

$$= \frac{1}{\sqrt{\pi \xi \hbar}} \int_{-\infty}^{\infty} y^2 \, e^{-\frac{y^2}{\xi\hbar}} \, dy$$

$$= \frac{1}{\sqrt{\pi \xi \hbar}} (\xi\hbar)^{3/2} \cdot 2 \int_0^{\infty} z^2 e^{-z^2} dz \rightarrow \frac{\sqrt{\pi}}{4}$$

$$= \frac{1}{2} \xi \hbar .$$

$$\Rightarrow \quad \xi = \frac{2}{\hbar} (\Delta x)^2 \quad \text{and} \quad N = \frac{1}{\sqrt[4]{2\pi (\Delta x)^2}}$$

So the spatial part of ψ looks like

$$\psi(x) = \frac{1}{(2\pi(\Delta x)^2)^{1/4}} \exp\left[- \frac{(x-\bar{x})^2}{4(\Delta x)^2} + \frac{i\bar{p}x}{\hbar} \right] .$$

Thus far, nothing at all has been mentionned about the Schrodinger eqn. It would be tempting to now assume that we can time evolve this result by simply appying a factor of

$$e^{-\frac{iEt}{\hbar}} \quad \text{with } E = \frac{\bar{p}^2}{2m} .$$

Of course, this won't work here because ψ is not

To be able to use the $e^{-\frac{iEt}{\hbar}}$ approach, we have to recast Ψ into momentum eigenstates:

$$u_k(x) = L^{-1/2} e^{ikx} \qquad \text{where } E = \frac{(\hbar k)^2}{2m}.$$

This comes from the normalization condition $\int_{-L/2}^{L/2} \psi^2 dx = 1$ where L is large.

If we write $\psi(r) = \sum_k A_k u_k(x)$

coefficients to be determined.

we will let this go to the continuum later

then $$\psi(r,t) = \sum_k A_k u_k(x) e^{-iE_k t/\hbar}$$

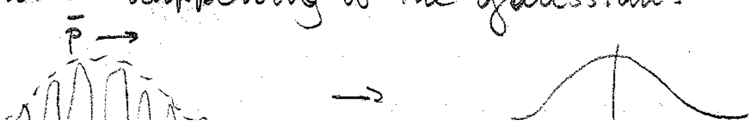
we can solve these at $t=0$ since norm is preserved.

With the definition of u_k used above,

$$A_k = \int u_k^*(x)\, \psi(x, t=0)\, dx$$

$$= \frac{1}{\sqrt{L}} \frac{1}{\sqrt[4]{2\pi(\Delta x)^2}} \int_{-L/2}^{L/2} \exp\left[-\frac{(x-\bar{x})^2}{4(\Delta x)^2} + i\left(\frac{\bar{p}}{\hbar} - k\right)x\right] dx$$

To make life a little simpler, let's put $\bar{x} = 0$ (i.e. put w.f on the origin) and $\bar{p} = 0$, so we're concentrating on what's happening to the gaussian.



$$A_k = \frac{1}{\sqrt[4]{2\pi (L\Delta x)^2}} \int_{-L/2}^{L/2} \exp\left[-\frac{x^2}{4(\Delta x)^2} - ikx\right] dx$$

$$= \underbrace{\frac{2\Delta x}{\sqrt[4]{2\pi L^2 \Delta x^2}}}_{\left(\frac{8\Delta x^2}{\pi L^2}\right)^{1/4}} \underbrace{\int_{-\frac{L}{4\Delta x}}^{\frac{L}{4\Delta x}} \exp\left[-y^2 - ik2\Delta x\, y\right] dy}_{\text{complete the square}} \qquad y = \frac{x}{2\Delta x}$$

$$\int_{-\frac{L}{4\Delta x}}^{\frac{L}{4\Delta x}} \exp\left[-\left(y^2 + 2(ik\Delta x)y + (ik\Delta x)^2 - (ik\Delta x)^2\right)\right] dy$$

$$= \int \exp\left[-(y + ik\Delta x)^2 - (k\Delta x)^2\right] dy$$

$$= e^{-(k\Delta x)^2} \int_{-\frac{L}{4\Delta x}+ik\Delta x}^{+\frac{L}{4\Delta x}+ik\Delta x} e^{-z^2} dz$$

$$= e^{-(k\Delta x)^2}\, 2 \cdot \frac{\sqrt{\pi}}{2}, \qquad \text{as } L \to \infty.$$

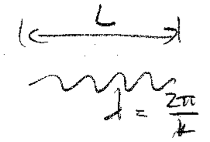
$$\therefore A_k = \left(\frac{8\Delta x^2}{\pi L^2}\right)^{1/4} \sqrt{\pi}\, e^{-k^2\Delta x^2} = \frac{1}{\sqrt{L}} (8\pi \Delta x^2)^{1/4} e^{-k^2 \Delta x^2}$$

So, using $\psi(x, t=0) = \sum_k A_k u_k$

$$= \sum_k (8\pi \Delta x^2)^{1/4} \frac{1}{\sqrt{L}} e^{-k^2\Delta x^2} \frac{1}{\sqrt{L}} e^{ikx}.$$

We want to go to the continuum limit of k.

Since $L = n\lambda = n\frac{2\pi}{k} \Rightarrow k = \frac{2\pi n}{L}$



or $\frac{dk}{dn} = \frac{2\pi}{L}$.

That is, the density of states is $\frac{2\pi}{L}$.

$$\text{So } \sum_k = \int \frac{L}{2\pi}\, dk .$$

This is Δn

$$\Rightarrow \psi(x, t=0) = \int dk \, \frac{L}{2\pi} (8\pi \Delta x^2)^{1/4} \frac{1}{L} e^{-k^2 \Delta x^2} e^{ikx}$$

$$= \left(\frac{\Delta x^2}{2\pi^3}\right)^{1/4} \int dk \, e^{-k^2 \Delta x^2} e^{ikx} .$$

For the time dependence, we get

$$\psi(x,t) = \left(\frac{\Delta x^2}{2\pi^3}\right)^{1/4} \int dk \, e^{-k^2 \Delta x^2} e^{ikx} e^{-\frac{i\hbar k^2 t}{2m}}$$

$$= \left(\frac{\Delta x^2}{2\pi^3}\right)^{1/4} \int dk \, \exp\Big[\underbrace{-\left(\Delta x^2 + \frac{i\hbar t}{2m}\right)k^2 + ikx}_{\text{This integral looks similar to what we had before.}}\Big]$$

$$y^2 = \left(\Delta x^2 + \frac{i\hbar t}{2m}\right)k^2$$

$$= \left(\frac{(\Delta x)^2}{2\pi^3}\right)^{1/4} \left(\Delta x^2 + \frac{i\hbar t}{2m}\right)^{-1/2} \int dy \, e^{-y^2 + ixy\left((\Delta x)^2 + \frac{i\hbar t}{2m}\right)^{-1/2}}$$

Integrate by completing the square

$$\int dy \, e^{-\left[y^2 - 2iy\frac{x\left(\Delta x^2 + \frac{i\hbar t}{2m}\right)^{-1/2}}{2} + \frac{i^2 x^2 \left(\Delta x^2 + \frac{i\hbar t}{2m}\right)^{-1}}{4} - \frac{i^2 x^2 \left(\Delta x^2 + \frac{i\hbar t}{2m}\right)^{-1}}{4}\right]}$$

$$= e^{\frac{i^2 x^2 \left(\Delta x^2 + \frac{i\hbar t}{2m}\right)^{-1}}{4}} \int e^{-\left(y - ix \frac{\left((\Delta x)^2 + \frac{i\hbar t}{2m}\right)^{-1/2}}{2}\right)^2} dy$$

$$= e^{-\frac{x^2}{4}\left(\Delta x^2 + \frac{i\hbar t}{2m}\right)^{-1}} \; 2 \cdot \frac{\sqrt{\pi}}{2}$$

$$\therefore \quad \psi(x,t) = \left(\frac{(\Delta x)^2}{2\pi^3}\right)^{1/4} \sqrt{\pi} \left(\Delta x^2 + \frac{i\hbar t}{2m}\right)^{-1/2} e^{-\frac{x^2}{4}\left(\Delta x^2 + \frac{i\hbar t}{2m}\right)^{-1}}$$

$$= \left(\frac{1}{2\pi}\right)^{1/4} \frac{(\Delta x)^{1/2}}{\left((\Delta x)^2 + \frac{i\hbar t}{2m}\right)^{1/2}} e^{-\left(\frac{x^2}{4\Delta x^2 + \frac{2i\hbar t}{m}}\right)}$$

Lastly, let's square all of this up to see how the density changes with time:

$$|\psi|^2 = \frac{1}{\sqrt{2\pi}} \frac{1}{\left(\Delta x + \frac{i\hbar t}{2m\Delta x}\right)^{1/2}} \frac{1}{\left(\Delta x - \frac{i\hbar t}{2m\Delta x}\right)^{1/2}} e^{-\left[\frac{x^2}{4(\Delta x)^2 + \frac{2i\hbar t}{m}} + \frac{x^2}{4(\Delta x)^2 - \frac{2i\hbar t}{m}}\right]}$$

$$= \left[(2\pi)\left[(\Delta x)^2 + \left(\frac{\hbar t}{2m\Delta x}\right)^2\right]\right]^{-1/2} \exp\left(-\frac{8(\Delta x)^2 x^2}{16(\Delta x)^4 + \frac{4\hbar^2 t^2}{m^2}}\right)$$

$$= \left[(2\pi)\left((\Delta x)^2 + \left(\frac{\hbar t}{2m\Delta x}\right)^2\right)\right]^{-1/2} \exp\left(-\frac{x^2}{2(\Delta x)^2 + \frac{1}{2}\left(\frac{\hbar t}{m\,\Delta x}\right)^2}\right)$$

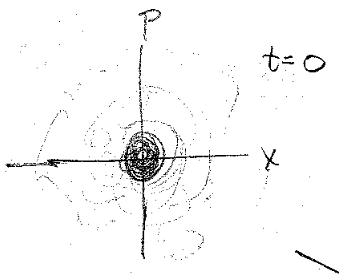
In other words, $|\psi|^2$ behaves like a gaussian with a time varying width given by

$$\sigma^2 = (\Delta x)^2 + \left(\frac{\hbar t}{2m\Delta x}\right)^2 .$$

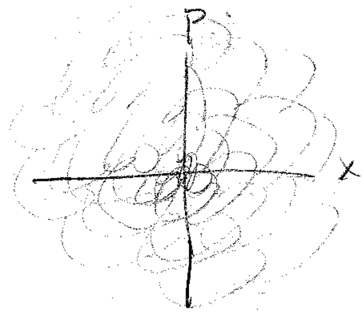
The physical significance of the width can be seen by substituting $\Delta x \cdot \Delta p = \frac{\hbar}{2}$.

$$\Rightarrow \quad \sigma^2 = (\Delta x)^2 + \left(\frac{\hbar t}{2m\frac{\hbar}{2\Delta p}}\right)^2 = (\Delta x)^2 + \left(\frac{\Delta p}{m} t\right)^2$$

velocity spread.



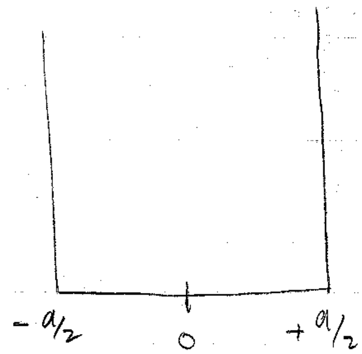
spread à la Liouville equ.



A summary of some simple problems evaluated in previous courses:

1. Infinite well:

$V(x) = 0 \quad -a/2 \leq x \leq a/2$
$V(x) = \infty$ otherwise.

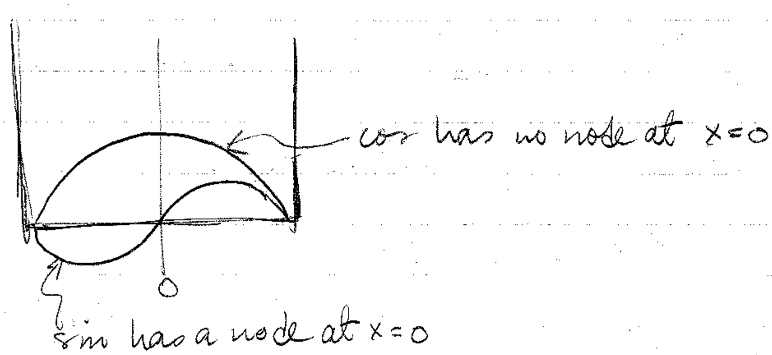


The 1-D Schrodingers equ. becomes

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = \epsilon\psi$$

As usual, we have two sets of solutions to this equation

$\psi \propto \cos(\cdots x) \qquad \psi \propto \sin(\cdots x)$.



The condition that $\psi \to 0$ at $x = \pm\frac{a}{2}$ is dictated by the requirement that the probability vanish in a region of infinite repulsive potential. This gives the usual quantization condition that