Time dependent Schrodinger eqn

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$$

Solution

$$|\psi(t)\rangle = e^{-\frac{iHt}{\hbar}}|\psi(0)\rangle$$

$$= \sum_n \underbrace{e^{-\frac{iHt}{\hbar}}|E_n\rangle}_{e^{-\frac{iE_nt}{\hbar}}|E_n\rangle}\underbrace{\langle E_n|\psi(0)\rangle}_{c_n(0)}$$

$$= \sum_n c_n(0)\, e^{-\frac{iE_nt}{\hbar}}|E_n\rangle$$

In position space

$$\langle x|\, i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = \langle x|H|\psi(t)\rangle$$

$$i\hbar \frac{\partial}{\partial t}\langle x|\psi(t)\rangle = H_{pos}\langle x|\psi(t)\rangle$$

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

usual t d S.e

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solution in position space

$$\psi(x,t) = \langle x|\psi(t)\rangle = \sum c_n(0)\, e^{-\frac{iE_nt}{\hbar}}\underbrace{\langle x|E_n\rangle}_{u_n(x)}$$

Coefficients of initial state

$$c_n(0) = \langle E_n|\psi(0)\rangle$$

$$= \int dx\, \langle E_n|x\rangle\langle x|\psi(0)\rangle$$

$$= \int dx\, u_n^*(x)\, \psi(x,0)$$

Time evolution of a square wave in a box.
Consider a particle of mass m in a one-dimensional box,

$$V(x) = \begin{cases} 0, & 0 < x < L \\ \infty, & \text{otherwise} \end{cases}$$

Suppose the wave-function of the particle at $t = 0$ is given by

$$\psi(x,0) = \begin{cases} \frac{1}{\sqrt{L}}, & 0 < x < L \\ 0, & \text{otherwise} \end{cases}$$

(Note: although this wavefunction is not continuous, you may consider it as a limiting case of a wavefunction that goes very quickly from 0 to $1/\sqrt{L}$ at the edges of the box.)

(a) If the energy of this particle were measured, what is the probability that you would obtain the ground state energy? What is the probability that you would obtain the first excited state energy?

(b) If the energy of the particle were not measured, compute $\psi(x,t)$, the wave-function of the particle at time t.

Time evolution of a free particle

$V(x) = V_0 = \text{const}$ (can set $= 0$)

$H = \frac{p^2}{2m} + V_0$

$\hat{H} = \frac{\hat{P}^2}{2m} + V_0 \hat{\mathbb{1}}$

momentum eigenstates $|p\rangle$ are also energy eigenstates

$\hat{H}\,|p\rangle = \left(\frac{p^2}{2m} + V_0\right)|p\rangle = E_p\,|p\rangle$

Expand $|\Psi(t)\rangle$ in momentum-space

$|\Psi(t)\rangle = \int dp \;\phi(p,t)\,|p\rangle$

$$\begin{aligned}
\phi(p,t) &= \langle p|\Psi(t)\rangle \\
&= \langle p|\, e^{-iHt/\hbar}\,|\Psi(0)\rangle \\
&= e^{-iE_pt/\hbar}\,\langle p|\Psi(0)\rangle \\
&= e^{-iE_pt/\hbar}\,\phi(p,0)
\end{aligned}$$

Momentum space probability density

$|\phi(p,t)|^2 = \left|e^{-iE_pt/\hbar}\,\phi(p,0)\right|^2 = |\phi(p,0)|^2$

independent of time!

$\Rightarrow \langle p\rangle, \langle p^2\rangle$, etc also indep of time

Position space wavepacket

$$|\psi(t)\rangle = \int dx \ \psi(x,t) \ |x\rangle$$

$$\psi(x,t) = \langle x | \psi(x,t)\rangle$$

$$= \langle x | e^{-\frac{iHt}{\hbar}} |\psi(0)\rangle$$

$$= \int dp \ \langle x|p\rangle \langle p| e^{-\frac{iHt}{\hbar}} |\psi(0)\rangle$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int dp \ e^{\frac{ipx}{\hbar}} \ e^{-\frac{iE_p t}{\hbar}} \ \underbrace{\langle p|\psi(0)\rangle}_{\phi(p,0)}$$

$$\underbrace{= \frac{1}{\sqrt{2\pi\hbar}} \int dp \ \phi(p,0) \ \underbrace{e^{\frac{ip}{\hbar}\left(x - \frac{E_p}{p} t\right)}}_{\text{travelling waves}}}_{\text{linear comb. of travelling waves} \ \equiv \ \text{"wave packet"}}$$

[phase velocity of travelling waves

$v_{ph} = \frac{E_p}{p}$ (different for diff p) dispersion

[www.eng.fsu.edu/~dommelen
gp vs phase velocity]

[group velocity of wave packet

$$v_{gp} = \frac{\partial E_p}{\partial p} = \frac{p}{m} = \text{classical velocity}$$

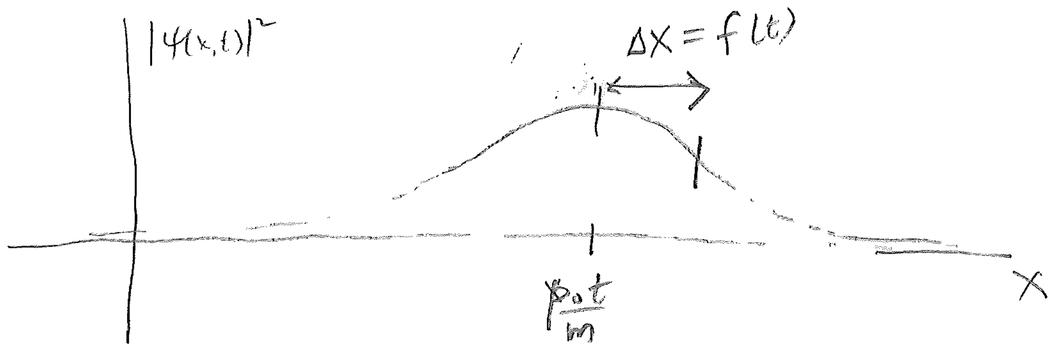
In HW, you will show that a gaussian distribution in momentum space

$$\phi(p,0) = \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} e^{-\beta(p-p_0)^2}$$

corresponds to a wave packet $\psi(x,t)$ whose probability density has the form

$$|\psi(x,t)|^2 = \sqrt{\frac{1}{2\pi f(t)^2}}\; e^{-\frac{(x-\frac{p_0}{m}t)^2}{2f(t)^2}}$$

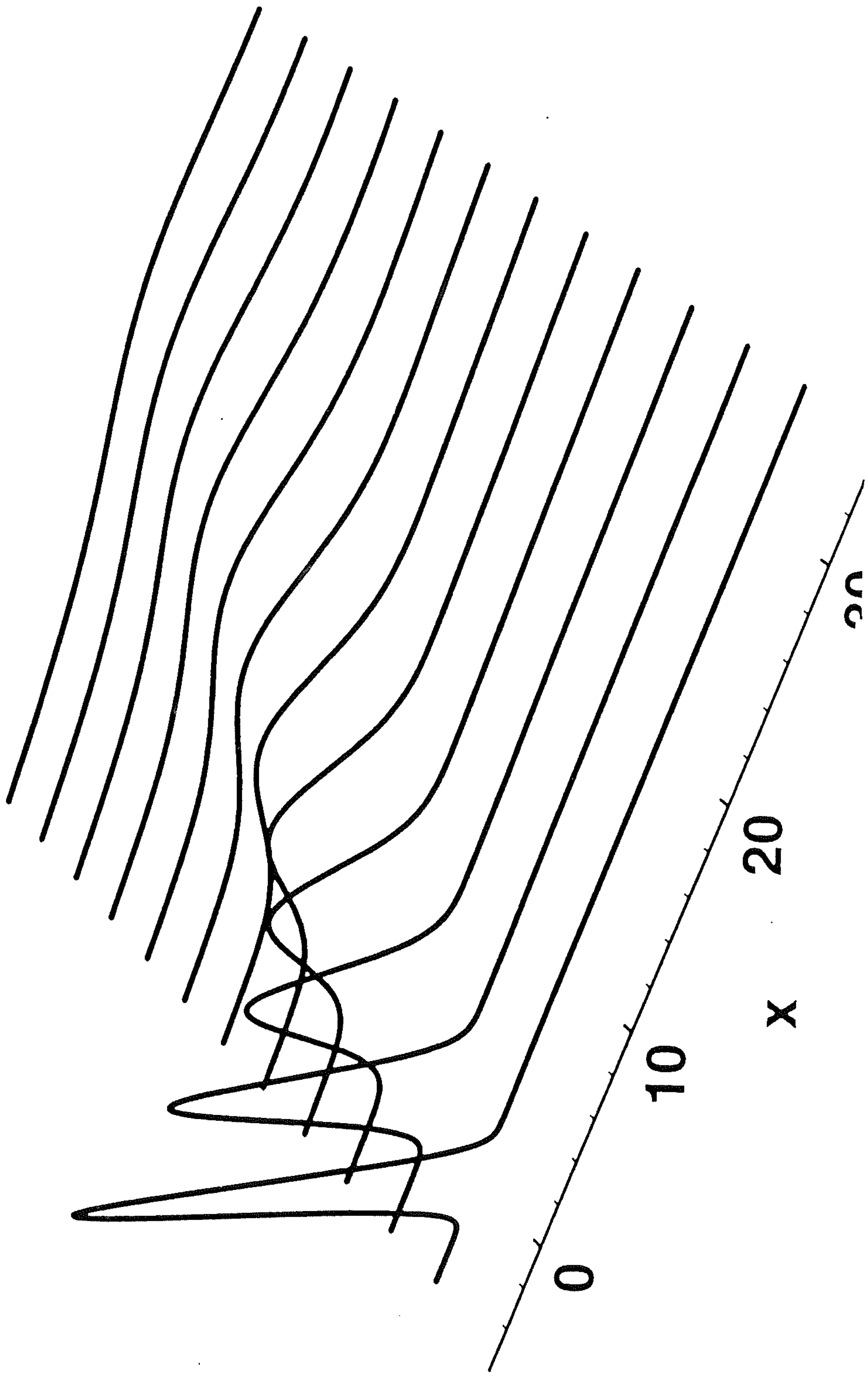
where $f(t)$ is a function that grows monotonically in time



This is a moving, spreading gaussian

- moves w/ speed $\frac{p_0}{m}$ = classical speed of particle
- uncertainty $\Delta x = f(t)$ increases in time.

QM. w/ Mathematica



Time evolution of a free Gaussian wavepacket.

(a) Consider a free particle, whose energy is given by $E_p = p^2/2m + V_0$ (with V_0 constant), and whose initial state at $t = 0$ is a Gaussian distribution in momentum space:

$$\phi(p,0) = \left(\frac{2\beta}{\pi}\right)^{1/4} \mathrm{e}^{-\beta(p-p_0)^2}$$

Show that the position-space wavefunction at time t is given by

$$\psi(x,t) = \left(\frac{2\beta}{\pi}\right)^{1/4} \left(\frac{1}{A+iB}\right)^{1/2} \mathrm{e}^{C+iD}$$

where A, B, C, and D are *real* expressions that you need to find.
[Hints: shift the variable of integration to $q = p - p_0$ before doing the integral. To deal with an expression of the form $1/(x+iy)$ in the exponent, multiply the exponent by $(x-iy)/(x-iy)$. Don't spend a lot of time simplifying D since it should drop out in the next step.]

(b) Show that the probability density of this wavefunction is

$$|\psi(x,t)|^2 = \left(\frac{1}{2\pi f(t)^2}\right)^{1/2} \exp\left(-\frac{(x-p_0t/m)^2}{2f(t)^2}\right)$$

and determine the form of the real function $f(t)$.

(c) Find $\langle p\rangle$, Δp, $\langle x\rangle$, and Δx at time t. (In particular, show that $\Delta x = f(t)$.) Since $f(t)$ is monotonically increasing with t, your solution describes a Gaussian in position space that is moving at constant speed, and spreading out as time goes on.

(d) Verify that the uncertainty principle holds for all values of t.

Free Gaussian wavepacket

We'll need $\int_{-\infty}^{\infty} dx\; e^{-ax^2 - by} = \sqrt{\frac{\pi}{a}}\; e^{\frac{b^2}{4a}}$

Given $\phi(p,0) = \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} e^{-\beta(p-p_0)^2}$

and $E_p = \frac{p^2}{2m} + V_0$

$$\phi(p,t) = \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} e^{-\beta(p-p_0)^2 - \frac{iE_p t}{\hbar}}$$

$$\psi(x,t) = \left(\frac{1}{2\pi\hbar}\right)^{\frac{1}{2}} \int dp\; e^{\frac{ipx}{\hbar}}\, \phi(p,t)$$

$$= \left(\frac{1}{2\pi\hbar}\right)^{\frac{1}{2}} \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \int dp\; e^{\frac{ipx}{\hbar}}\, e^{-\beta(p-p_0)^2}\, e^{-\frac{itp^2}{2\hbar m}}\, e^{-\frac{iV_0 t}{\hbar}}$$

$$= \left(\frac{1}{2\pi\hbar}\right)^{\frac{1}{2}} \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \int dq\; e^{\frac{i(p_0+q)x}{\hbar}}\, e^{-\beta q^2}\, e^{-\frac{it}{2\hbar m}(p_0^2 + 2p_0 q + q^2)}\, e^{-\frac{iV_0 t}{\hbar}}$$

$$= \left(\frac{1}{2\pi\hbar}\right)^{\frac{1}{2}} \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \int dq\; e^{-aq^2 - bq - c}$$

where
$$\begin{cases} a = \beta + \frac{it}{2\hbar m} = \frac{1}{2\hbar m}\left(2\hbar m\beta + it\right) \\ b = -\frac{ix}{\hbar} + \frac{itp_0}{\hbar m} = -\frac{i}{\hbar}\left(x - \frac{p_0 t}{m}\right) \\ c = -\frac{ip_0 x}{\hbar} + \frac{itp_0^2}{2\hbar m} + \frac{iV_0 t}{\hbar} \end{cases}$$

Now $$\frac{b^2}{4a} = \frac{\left(-\frac{i}{\hbar}\right)^2 \left(x - \frac{p_0 t}{m}\right)^2}{\frac{2}{\hbar m}\left(2\hbar m\beta + it\right)} \frac{\left(2\hbar m\beta - it\right)}{\left(2\hbar m\beta - it\right)}$$

$$= -\frac{m}{2\hbar} \frac{\left(x - \frac{p_0 t}{m}\right)^2 \left(2\hbar m\beta - it\right)}{\left(4\hbar^2 m^2\beta^2 + t^2\right)}$$

Thus

$$\psi(x,t) = \left(\frac{1}{2\pi\hbar}\right)^{\frac{1}{2}} \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \left(\frac{2\pi\hbar m}{2\hbar m\beta + it}\right)^{\frac{1}{2}} e^{-\frac{m}{2\hbar}\frac{\left(x - \frac{p_0 t}{m}\right)^2\left(2\hbar m\beta - it\right)}{\left(4\hbar^2 m^2\beta^2 + t^2\right)} - c}$$

$$= \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \left(\frac{1}{2\hbar\beta + i\frac{t}{m}}\right)^{\frac{1}{2}} e^{-\frac{\left(x - \frac{p_0 t}{m}\right)^2\left(m^2\beta - \frac{imt}{2\hbar}\right)}{\left(4\hbar^2 m^2\beta^2 + t^2\right)} - c}$$

$$= \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \left(\frac{1}{A + iB}\right)^{\frac{1}{2}} e^{C + iD}$$

where

$$\begin{cases} A = 2\hbar\beta \\ B = \frac{t}{m} \\ C = -\frac{m^2\beta}{\left(4\hbar^2 m^2\beta^2 + t^2\right)}\left(x - \frac{p_0}{m}t\right)^2 \\ D = \frac{mt\left(x - \frac{p_0}{m}t\right)^2}{2\hbar\left(4\hbar^2 m^2\beta^2 + t^2\right)} + \frac{p_0 x}{\hbar} - \frac{p_0^2 t}{2\hbar m} - \frac{V_0 t}{\hbar} \end{cases}$$

[Although this is unnecessary, D can be simplified to

$$D = \frac{\frac{mt}{2\hbar}x^2 + 4\hbar\beta^2 m^2 p_0 x - 2\hbar\beta^2 m p_0^2 t}{\left(4\hbar^2 m^2\beta^2 + t^2\right)} - \frac{V_0 t}{\hbar}$$]

It is a little harder to do the integrals w/o shifting first (3)

$$\int_{-\infty}^{\infty} dx\, e^{-ax^2 - bx - c} = \sqrt{\frac{\pi}{a}}\, e^{\frac{b^2}{4a} - c}$$

$$\psi(x,t) = \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \left(\frac{1}{2\pi\hbar}\right)^{\frac{1}{2}} \int dp\, e^{\frac{ipx}{\hbar}} e^{-\beta(p-p_0)^2} e^{-\frac{it}{2\hbar m}p^2} e^{-\frac{iV_0 t}{\hbar}}$$

$$= \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \left(\frac{1}{2\pi\hbar}\right)^{\frac{1}{2}} \int dp\, e^{-ap^2 - bp - c}$$

where
$$\begin{cases} a = \beta + \frac{it}{2\hbar m} = \frac{1}{2\hbar m}(2\hbar m\beta + it) \\ b = -\frac{ix}{\hbar} - 2\beta p_0 \\ c = \beta p_0^2 + \frac{iV_0 t}{\hbar} \end{cases}$$

$$\frac{b^2}{4a} = \frac{\left(-\frac{1}{\hbar}\right)^2 (ix + 2\hbar\beta p_0)^2 (2\hbar m\beta - it)}{\left(\frac{2}{\hbar m}\right)(2\hbar m\beta + it)(2\hbar m\beta - it)}$$

$$= \frac{m}{2\hbar} \frac{(-x^2 + 4i\hbar\beta x p_0 + 4\hbar^2\beta^2 p_0^2)(2\hbar m\beta - it)}{(4\hbar^2 m^2\beta^2 + t^2)}$$

$$= \frac{m}{2\hbar} \frac{\left(-2\hbar m\beta x^2 + 8\hbar^3 m\beta^3 p_0^2 + 4\hbar\beta p_0 x t + i(x^2 t - 4\hbar^2\beta^2 p_0^2 t + 8\hbar^2 m\beta^2 x p_0)\right)}{(4\hbar^2 m^2\beta^2 + t^2)}$$

To this we add $\quad -c = \dfrac{-4\hbar^2 m^2\beta^3 p_0^2 - \beta p_0^2 t^2}{4\hbar^2 m^2\beta^2 + t^2} - \dfrac{iV_0 t}{\hbar}$

to obtain:

$$\frac{-m^2\beta\left(x^2 - 2\frac{p_0}{m}xt + \frac{p_0^2 t^2}{m^2}\right)}{(4\hbar^2 m^2\beta^2 + t^2)} + i\left[\frac{\frac{mtx^2}{2\hbar} + 4\hbar m^2\beta^2 x p_0 - 2\hbar\beta^2 m p_0^2 t}{(4\hbar^2 m^2\beta^2 + t^2)} - \frac{V_0 t}{\hbar}\right]$$

which is precisely $C + iD$ obtained before

$$|\psi(x,t)|^2 = \left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}} \left(\frac{1}{A^2+B^2}\right)^{\frac{1}{2}} e^{2C}$$

where $$2C = -\frac{2m^2\beta}{4\hbar^2 m^2\beta^2 + t^2}\left(x - \frac{p_0}{m}t\right)^2$$

$$= \frac{-\left(x - \frac{p_0}{m}t\right)^2}{2\left(\hbar^2\beta + \frac{t^2}{4m^2\beta}\right)}$$

and

$$\frac{2\beta}{\pi(A^2+B^2)} = \frac{2\beta}{\pi\left(4\hbar^2\beta^2 + \frac{t^2}{m^2}\right)} = \frac{1}{2\pi\left(\hbar^2\beta + \frac{t^2}{4m^2\beta}\right)}$$

Thus

$$|\psi(x,t)|^2 = \left(\frac{1}{2\pi f^2}\right) e^{-\frac{\left(x - \frac{p_0 t}{m}\right)^2}{2f^2}}$$

where $$\boxed{f(t) = \sqrt{\hbar^2\beta + \frac{t^2}{4m^2\beta}}}$$

(c)

$$\langle p \rangle = p_0$$

$$\Delta p = \frac{1}{\sqrt{4\beta}}$$

These are independent of time, as shown in class

$$\langle x \rangle = \frac{p_0 t}{m}$$

$$\Delta x = \frac{1}{\sqrt{4\alpha}} = f(t)$$

$$e^{-2\alpha(x-x_0)^2} = e^{-\frac{(x-\frac{p_0 t}{m})^2}{2f^2}}$$

$$\alpha = \frac{1}{4f^2}$$

(d)

$$\Delta x \, \Delta p = \frac{f(t)}{\sqrt{4\beta}} = \sqrt{\frac{\hbar^2}{4} + \frac{t^2}{16 m^2 \beta^2}}$$

$$= \sqrt{\left(\frac{\hbar}{2}\right)^2 + \left(\frac{t}{4m\beta}\right)^2}$$

$$= \frac{\hbar}{2}\sqrt{1 + \left(\frac{t}{2\hbar m\beta}\right)^2}$$

$$\geq \frac{\hbar}{2}$$