2.4 The free particle

The free particle has V(x)=0 everywhere. Classically, it is easy to solve, such as a ball moving straight in empty space. However, in QM it is more subtle and complicated.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad \text{or} \quad \frac{d^2\psi}{dx^2} = -k^2\psi \quad \text{with} \quad k \equiv \frac{\sqrt{2mE}}{\hbar}$$

(E>0)

If you try $\psi(x) = Ae^{ikx} + Be^{-ikx}$ it works.

k, and thus *E*, are unrestricted since there is no boundary.
No discrete levels but a continuum of levels.

Adding time dependence, it becomes:

$$\Psi(x,t) = Ae^{ik\left(x-\frac{\hbar k}{2m}t\right)} + Be^{-ik\left(x+\frac{\hbar k}{2m}t\right)}$$

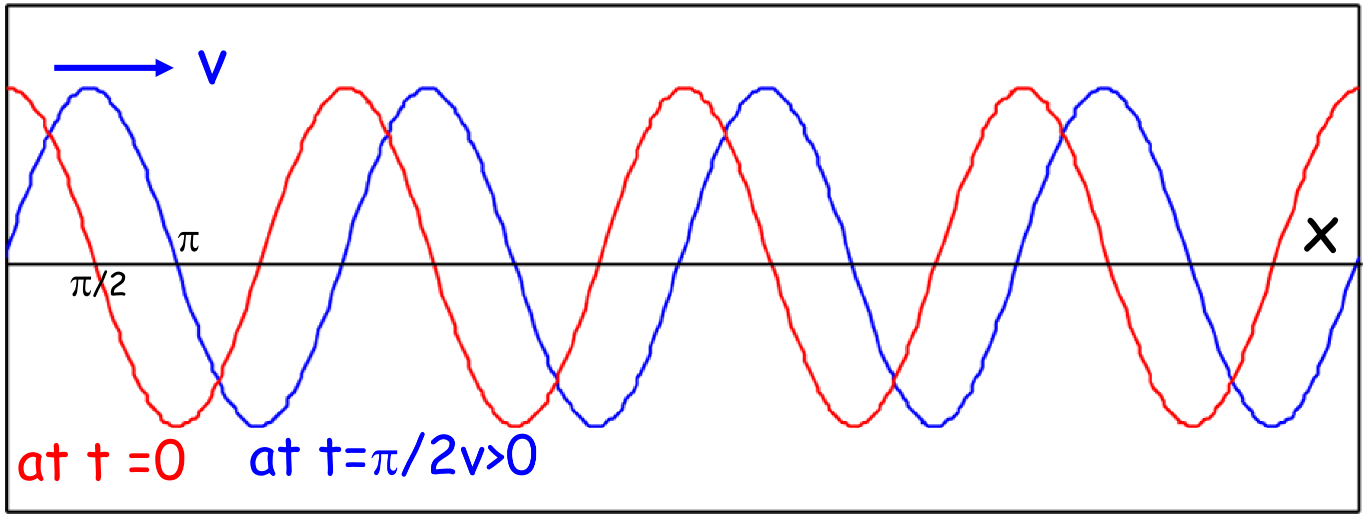
where $E = \hbar^2k^2/2m$

Introduce v = $\hbar k/2m$ as a velocity (check units!)

Then, in exponents we have $(x \pm vt)$

cos(x-vt)

with "-vt" moves to the right



$\xrightarrow{\quad\quad}$ v $\quad\quad$ $\xleftarrow{\quad\quad}$ -v

$$\Psi(x,t) = Ae^{ik(x-\boxed{\frac{\hbar k}{2m}}t)} + Be^{-ik(x+\boxed{\frac{\hbar k}{2m}}t)}$$

Compact form:

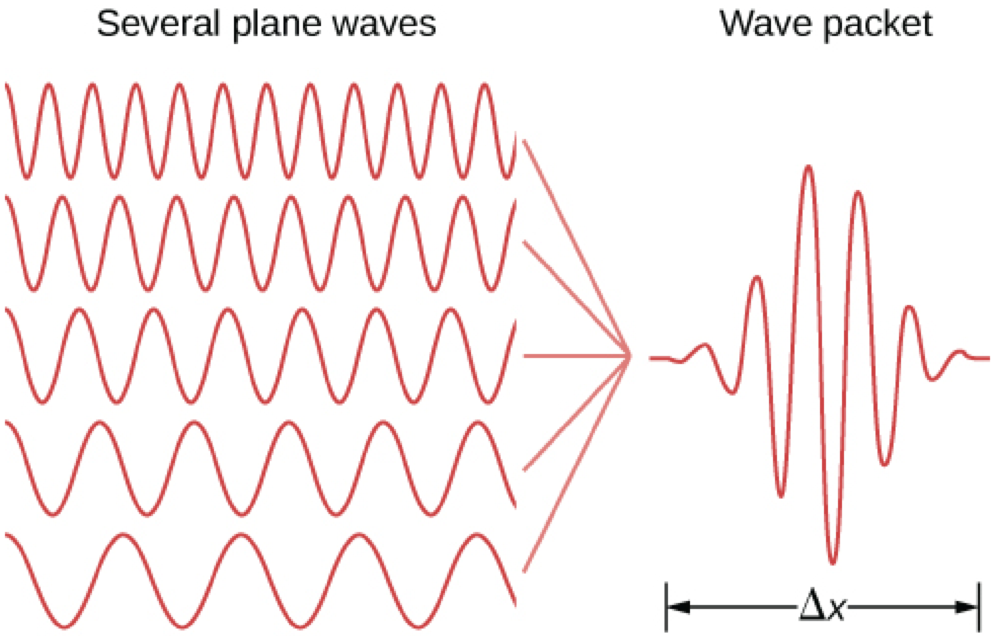
$$\boxed{\Psi_k(x,t) = A_k e^{i(kx-\frac{\hbar k^2}{2m}t)} \quad \text{with } k \equiv \pm\frac{\sqrt{2mE}}{\hbar}}$$

Two paradoxes:

$v = \hbar k/2m = p/2m$ (after using de Broglie formula) $= \frac{1}{2}$ classical formula $v=p/m$

Solutions are not normalizable because $\Psi^*\Psi=1$ for all x, thus integral over x diverges: no stationary states for free particles. ☹

We can “solve” this problem via wave packets (i.e. linear combination of plane waves).



Note Δx is **not** size of electron which remains point-like when measured.

Because *k* is unrestricted, linear combinations are integrals instead of sums.

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i\left(kx - \frac{\hbar k^2}{2m} t\right)}\, dk$$

$(1/\sqrt{2\pi})\phi(k)\, dk$ is like c_n in $\underbrace{\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-i(n^2\pi^2\hbar/2ma^2)t}}_{\text{infinite square well as example}}$

Like before, we are given the *t=0* wave function and from there we must find $\phi(k)$.

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{ikx}\, dk$$

In a typical problem this is provided

unknown

We use Fourier analysis (page 56) to find $\phi(k)$.

$$\boxed{f(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}F(k)e^{ikx}\,dk \Longleftrightarrow F(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}f(x)e^{-ikx}\,dx}$$

Inverse Fourier transform

Fourier transform of f(x)

Applied to our problem, the formula to use is:

unknown

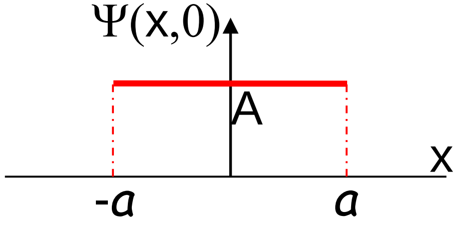
provided

$$\boxed{\phi(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\Psi(x,0)e^{-ikx}\,dx}$$

Problem 2.20b

Analog of $c_n=\sqrt{\frac{2}{a}}\int_0^a \sin\left(\frac{n\pi}{a}x\right)\Psi(x,0)\,dx$ for sq. well.

Example 2.6: evolution of a localized t=0 state



Given $\Psi(x,0) = \begin{cases} A, & \text{if } -a < x < a, \\ 0, & \text{otherwise,} \end{cases}$ find $\Psi(x,t)$

First step: normalization at t=0

$$1 = \int_{-\infty}^{\infty} |\Psi(x,0)|^2\,dx = |A|^2 \int_{-a}^{a} dx = 2a|A|^2 \Rightarrow \boxed{A = \frac{1}{\sqrt{2a}}}$$

Second, calculate $\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,0)e^{-ikx}\,dx$

$$\phi(k) = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2a}} \int_{-a}^{a} e^{-ikx}\,dx = \frac{1}{2\sqrt{\pi a}} \frac{e^{-ikx}}{-ik}\Bigg|_{-a}^{a}$$

$$= \frac{1}{k\sqrt{\pi a}}\left(\frac{e^{ika} - e^{-ika}}{2i}\right) = \boxed{\frac{1}{\sqrt{\pi a}}\frac{\sin(ka)}{k}}.$$

Check every step!

Third, and last, use $\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m} t)}\, dk$

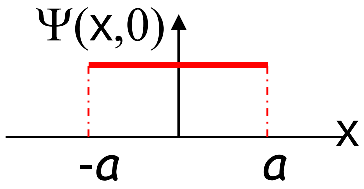
$$\boxed{\Psi(x,t) = \frac{1}{\pi\sqrt{2a}} \int_{-\infty}^{\infty} \frac{\sin(ka)}{k} e^{i(kx - \frac{\hbar k^2}{2m} t)}\, dk}$$

previous page (helps also for prob. 2.20c)

$$\frac{\phi(k)}{\sqrt{2\pi}}$$

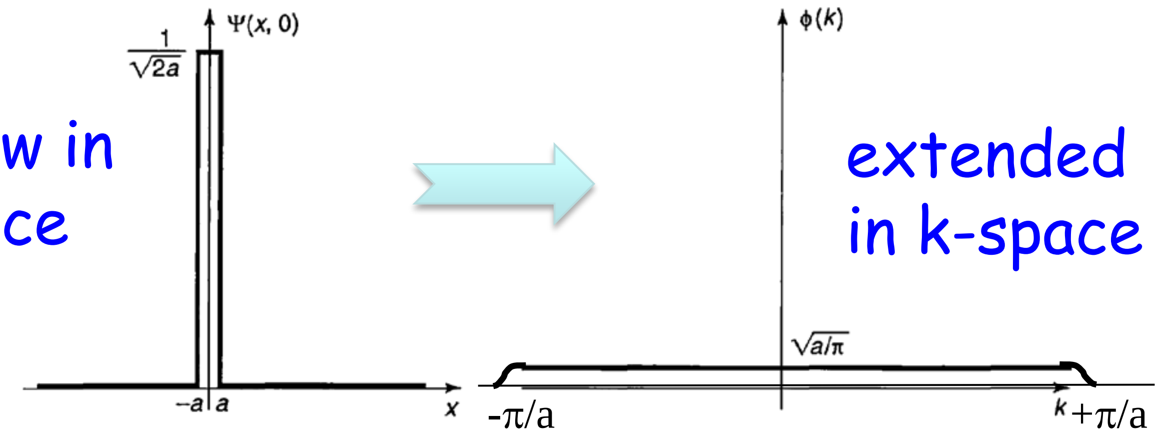
This integral must be computed numerically, although special limits can be done analytically.

(1) *If a* is small, then *t=0* state is **localized in space**



$$\phi(k) = \frac{1}{\sqrt{\pi a}} \frac{\sin(ka)}{k} \approx \sqrt{\frac{a}{\pi}}$$

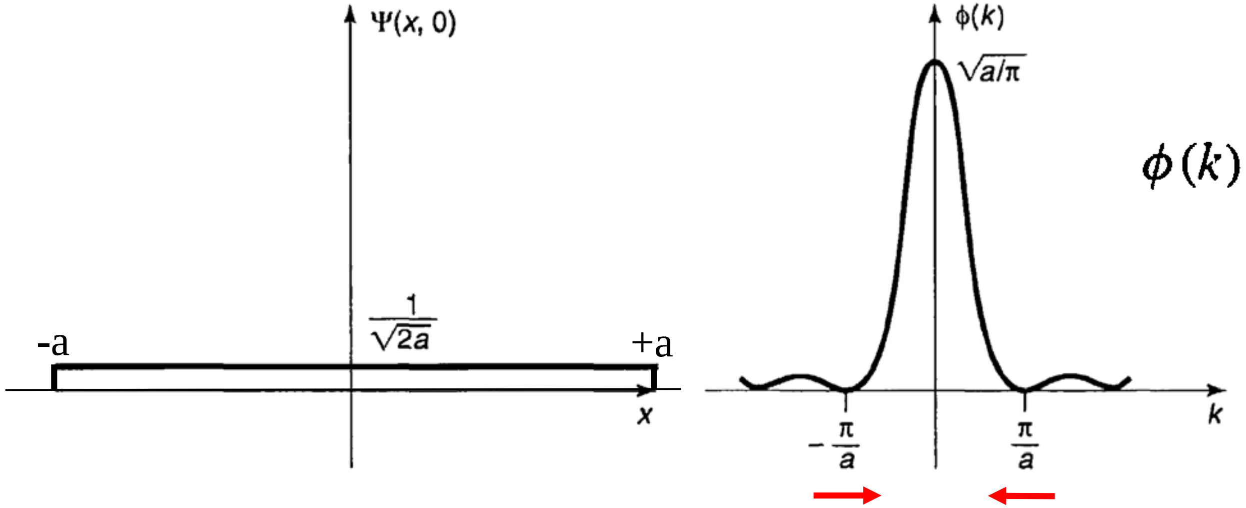
$\sin(ka) \approx ka$



narrow in x-space

extended in k-space

(2) ***If a* is large**, then t=0 state is **spread in space**

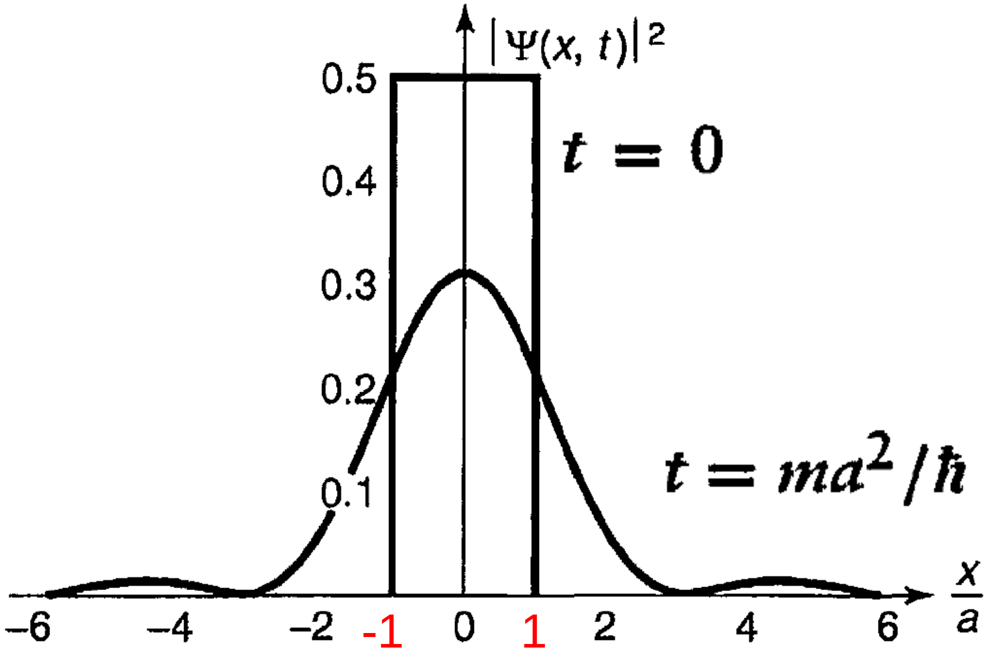


$$\phi(k) = \frac{1}{\sqrt{\pi a}} \frac{\sin(ka)}{k}$$

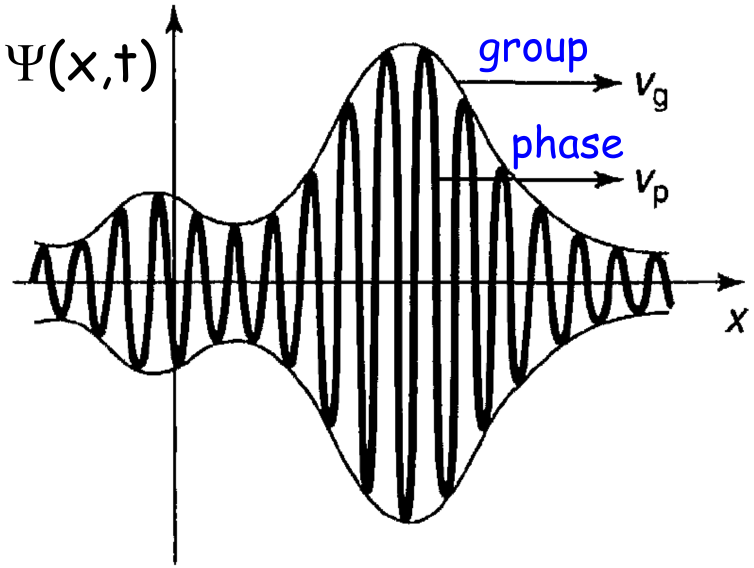
Sharp peak as “a” grows

Returning to $\Psi(x,t) = \frac{1}{\pi\sqrt{2a}} \int_{-\infty}^{\infty} \frac{\sin(ka)}{k} e^{i(kx - \frac{\hbar k^2}{2m} t)}\, dk$

and numerically calculating integral leads to spreading of initial state (general: width increases as time increases)



The paradox v=(1/2) p/m can be addressed in the context of wave packets. The speed of the sinusoidal components (phase velocity) is not important. The envelope's speed (group velocity) is more relevant. Movies coming soon..



$\omega = (\hbar k^2/2m)$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)e^{i(kx-\omega t)}\,dk.$$

Assume $\phi(k)$ is narrowly peaked $k=k_0+s$. Thus, $k^2 \sim k_0^2 + 2k_0s$ (where s^2 was dropped).

$\hbar k_0^2/2m$ $\hbar k_0/m$

$$\Psi(x,t) \cong \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k_0+s)e^{i[(k_0+s)x-(\omega_0+\omega_0' s)t]}\,ds$$

Drop s^2 term

$$\Psi(x,t) \cong \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_0+s)\, e^{i[(k_0+s)x-(\omega_0+\omega_0' s)t]}\, ds$$

Moves outside integral

$-\omega_0'st = -\omega_0'st + k_0\omega_0't - k_0\omega_0't =$

$= + k_0\omega_0't - (k_0+s)\,\omega_0't$

Then

$$\Psi(x,t) \cong \frac{1}{\sqrt{2\pi}} e^{i(-\omega_0 t + k_0\omega_0' t)} \int_{-\infty}^{+\infty} \phi(k_0+s)\, e^{i(k_0+s)(x-\omega_0' t)}\, ds$$

Because

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_0+s)\, e^{i(k_0+s)x}\, ds.$$

then

$$\Psi(x,t) \cong \underbrace{e^{-i(\omega_0-k_0\omega_0')t}}_{\text{Not important for } |\Psi|^2}\, \underbrace{\Psi(x-\omega_0't,\, 0)}_{\text{Same shape as original wave packet but moving!}}$$

$\omega_0' = \hbar k_0/m = p_0/m$

velocity of wave packet

Velocity of wave packet is correctly $v_{\text{classical}}$!