To prepare for Test 1 Sept 24,
drop problems 1.3, 1.7, 1.8 from HW1.

2.4 The free particle

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

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

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

k, and thus *E*, are unrestricted since there is no boundary.

Adding time dependence it becomes:

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

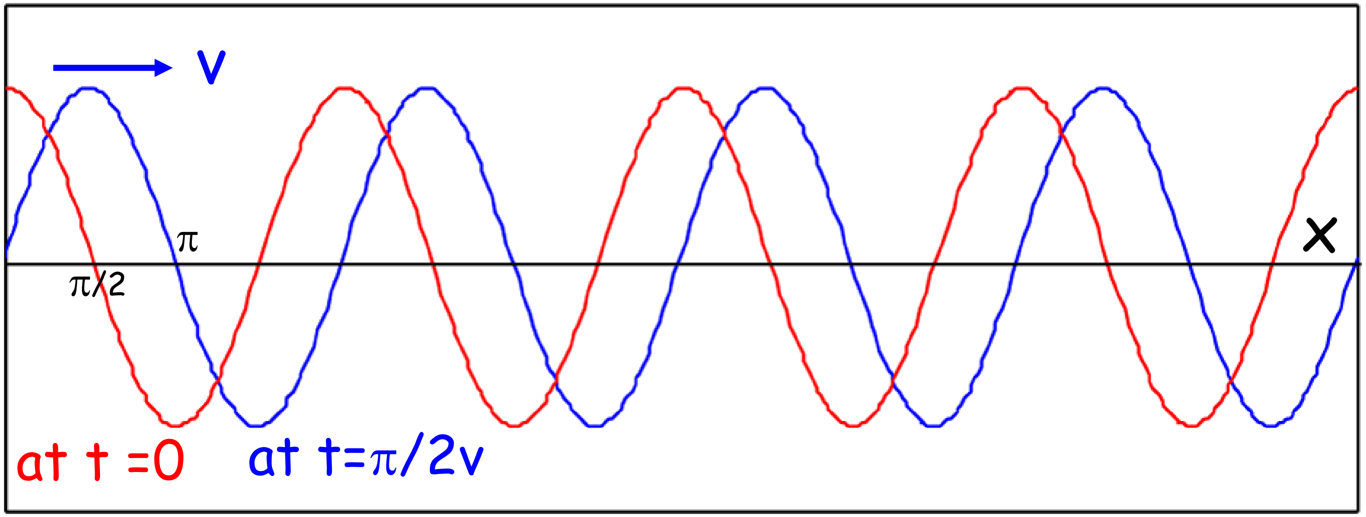
where $E = \hbar^2 k^2 / 2m$

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

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

cos(x-vt)

"-vt" term moves to the right



v → ← -v

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

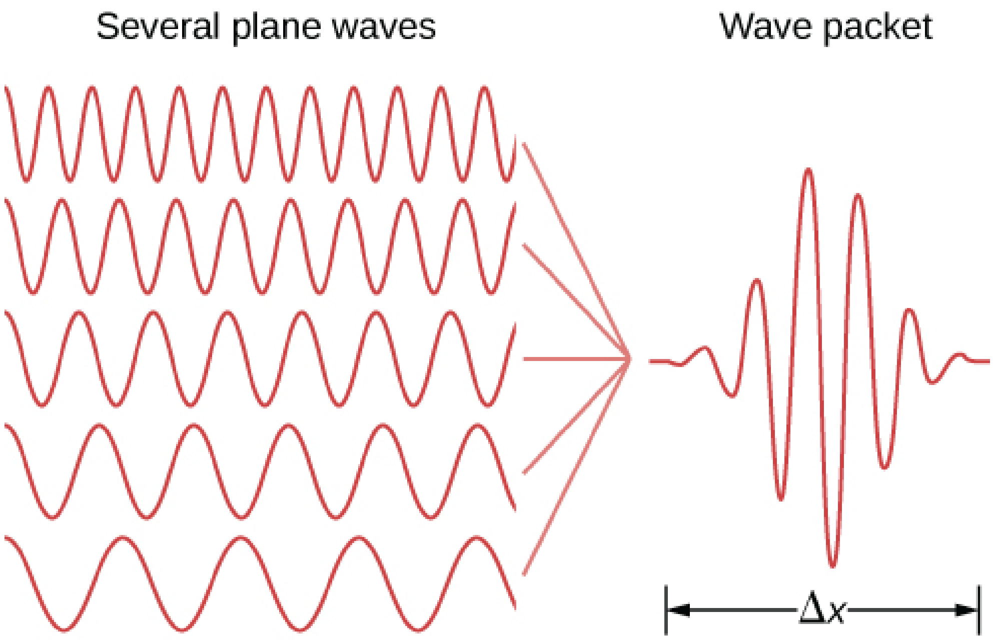
Compact form:

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

Two paradoxes:

$v = \hbar k/2m = p/2m$ (using de Broglie formula) = ½ 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).

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 $\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-i(n^2\pi^2\hbar/2ma^2)t}$

infinite square well as example

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

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

provided — unknown

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

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

Inverse Fourier transform — Fourier transform of f(x)

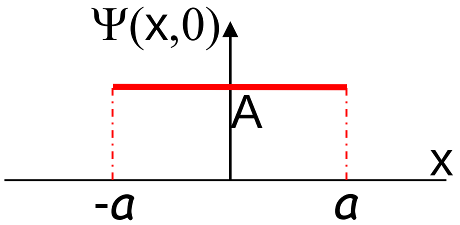
Applied to our problem, the formula to use is:

unknown — provided

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

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

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

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

Check every step!

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

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

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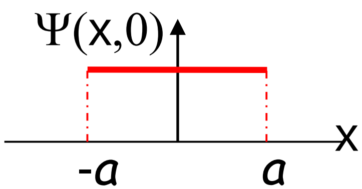
$$\frac{\phi(k)}{\sqrt{2\pi}}$$

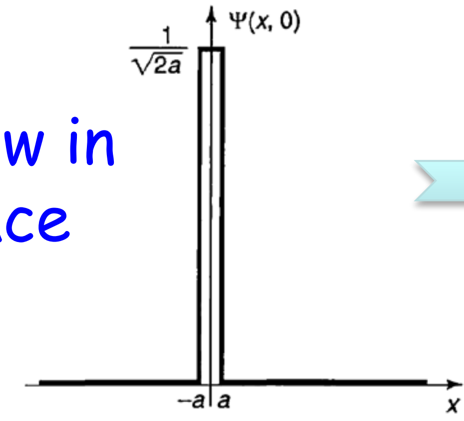
This integral must be computed numerically, although special limits can be done analytically.

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

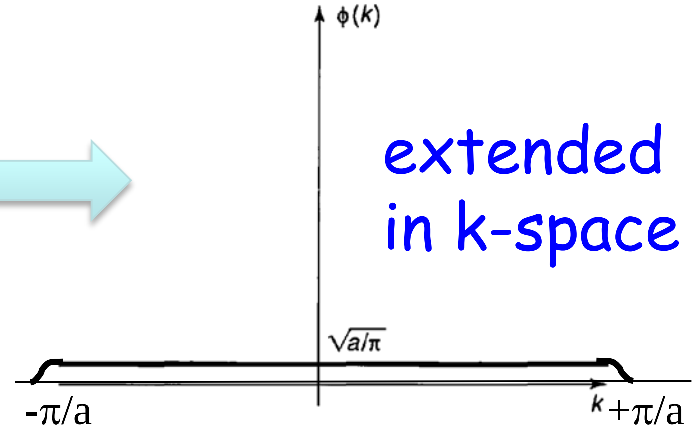


$$\phi(k) = \frac{1}{\sqrt{\pi a}} \frac{\sin(ka)}{k} \approx \sqrt{\frac{a}{\pi}}$$

$\sin(ka) \approx ka$

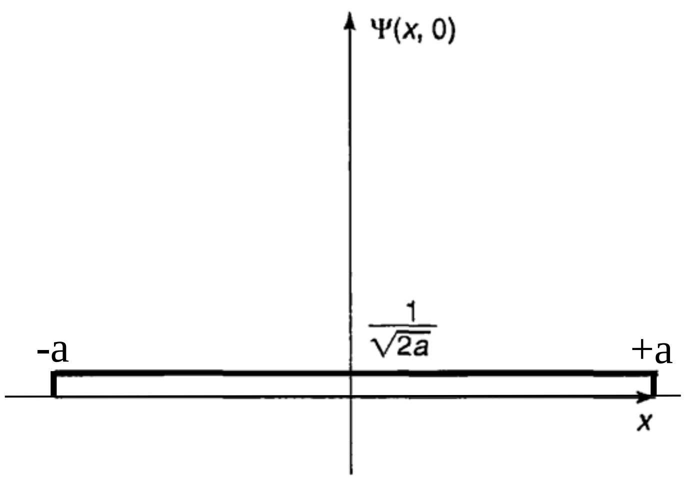


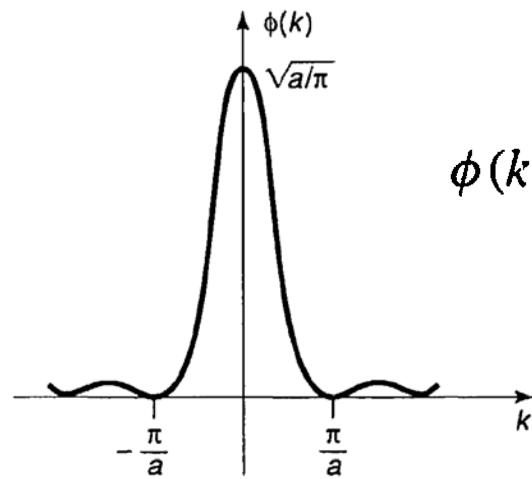
narrow in x-space



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