

The free particle

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

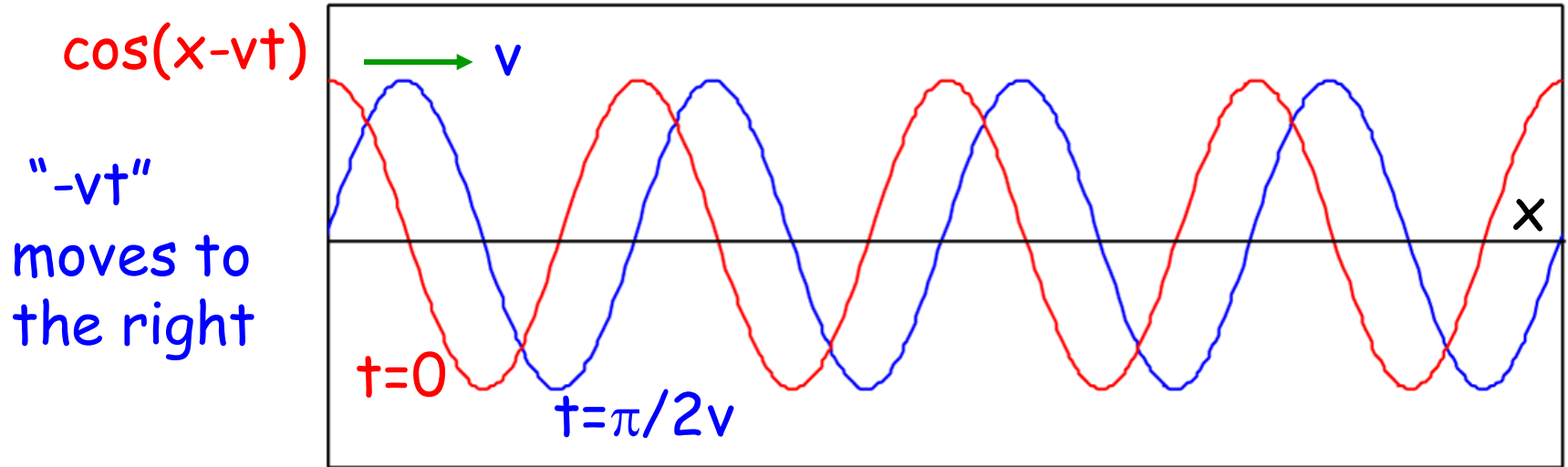
Adding time dependence it becomes:

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

$$\text{where } E = \hbar^2 k^2 / 2m$$

Introduce $v = \hbar k/2m$ as a velocity

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



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

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

Compact form:

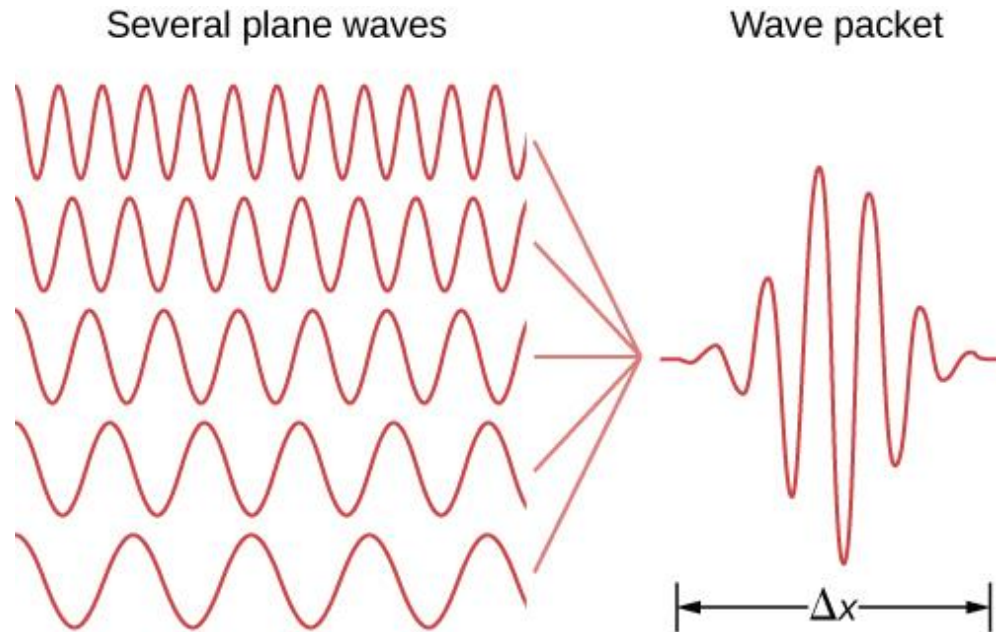
$$\Psi_k(x, t) = Ae^{i(kx - \frac{\hbar k^2}{2m}t)} \quad \text{with } k \equiv \pm \frac{\sqrt{2mE}}{\hbar}$$

Two paradoxes:

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

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

Wave packets (i.e. linear combination of plane waves) saves the day!



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

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

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

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

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

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

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

Inverse Fourier transform

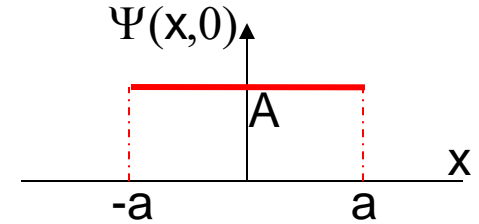
Fourier transform

Applied to our problem, the formula to use is:

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

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: 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 $t=0$

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

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

$$\begin{aligned} \phi(k) &= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2a}} \int_{-a}^a e^{-ikx} dx = \frac{1}{2\sqrt{\pi a}} \frac{e^{-ikx}}{-ik} \Big|_{-a}^a \\ &= \frac{1}{k\sqrt{\pi a}} \left(\frac{e^{ika} - e^{-ika}}{2i} \right) = \frac{1}{\sqrt{\pi a}} \frac{\sin(ka)}{k}. \end{aligned}$$

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

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

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

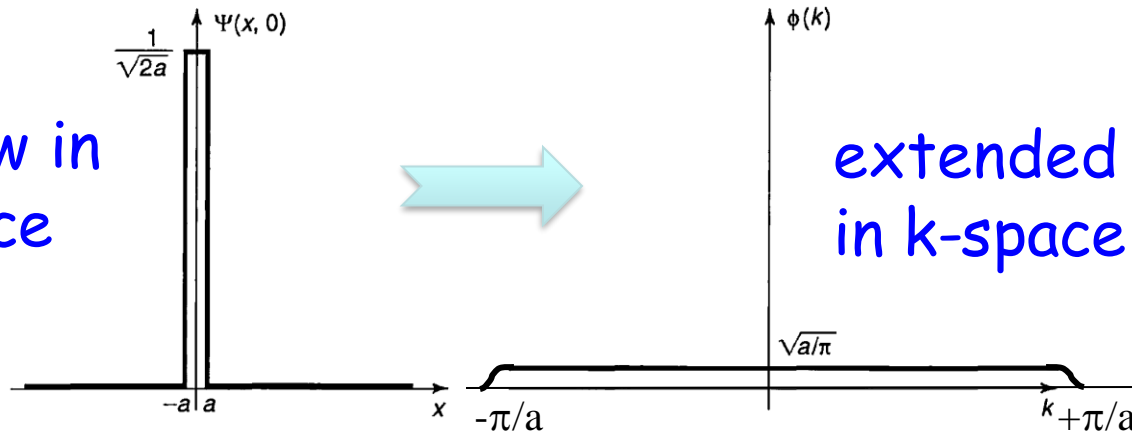
This integral must be computed **numerically**, although special limits can be done by hand.

(1) a is small, thus $t=0$ state is very localized

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

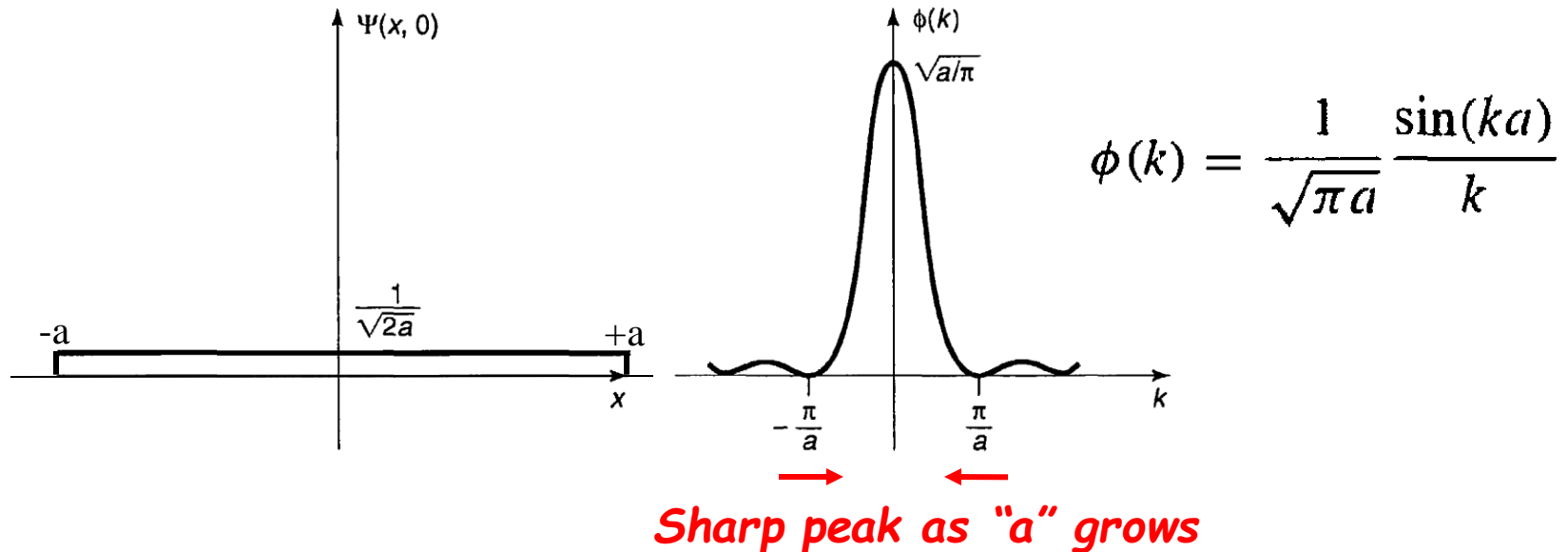
$\sin(ka) \approx ka$

narrow in
x-space



extended
in k-space

(2) a is large, thus $t=0$ state is very spread



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 solving the problem leads to spreading of initial state (width increases as time increases)

