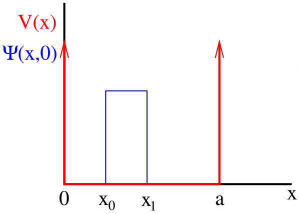
Making Movies - Time Development

Recall the rectangular initial wave packet in the infinite square well shown below. How does it evolve in time?

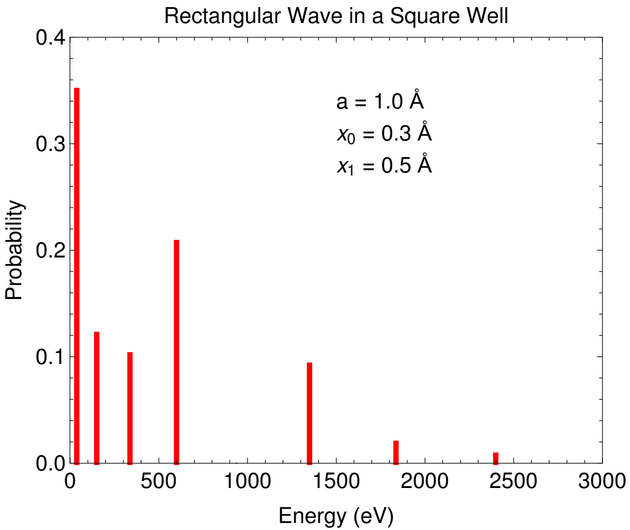
$$
\begin{aligned}
V(x) &= 0 \qquad 0 < x < a \\
&= \infty \qquad x \leq 0 \quad \text{and} \quad x \geq a
\end{aligned}
$$

$$
\begin{aligned}
|\Psi(x,0)\rangle &= \frac{1}{\sqrt{d}} \quad x_0 \leq x \leq x_1 \quad \text{and} \quad d = x_0 - x_1 \\
&= 0 \qquad \text{otherwise}
\end{aligned}
$$

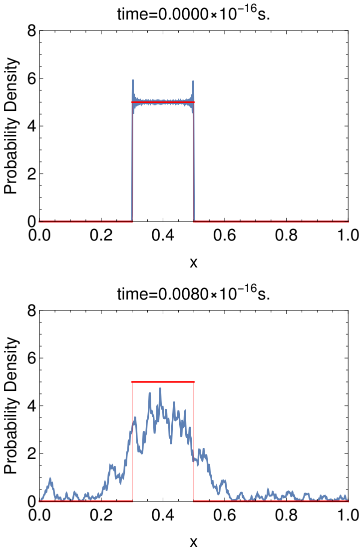


$$
\begin{aligned}
a &= 1.0 \text{ Å} \\
x_0 &= 0.3 \text{ Å} \\
x_1 &= 0.5 \text{ Å}
\end{aligned}
$$

Probabilities of Different States



Time Development of a Square Wave



Comparison of Bound and Free Particles

Particle in a Box

The potential

$$\begin{aligned} V =& 0 \qquad 0 < x < a \\ =& \infty \qquad \textit{otherwise} \end{aligned}$$

Eigenfunctions and eigenvalues

$$|\phi_n\rangle = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \qquad E_n = n^2 \frac{\hbar^2 \pi^2}{2ma^2}$$

Superposition

$$|\psi\rangle = \sum_{n=1}^{\infty} b_n |\phi_n\rangle \qquad \langle \phi_m | \phi_n \rangle = \delta_{m,n}$$

Getting the coefficients

$$b_n = \langle \phi_n | \psi \rangle \qquad P_n = |b_n|^2$$

Free Particle

The potential

$$V = 0$$

Eigenfunctions and eigenvalues

$$|\phi(k)\rangle = \frac{1}{\sqrt{2\pi}} e^{\pm ikx} \qquad E = \frac{\hbar^2 k^2}{2m}$$

Superposition

$$\begin{aligned} |\psi\rangle =& \int_{-\infty}^{\infty} b(k)\phi(k) dk \\ \langle \phi(k') | \phi(k) \rangle =& \delta(k - k') \end{aligned}$$

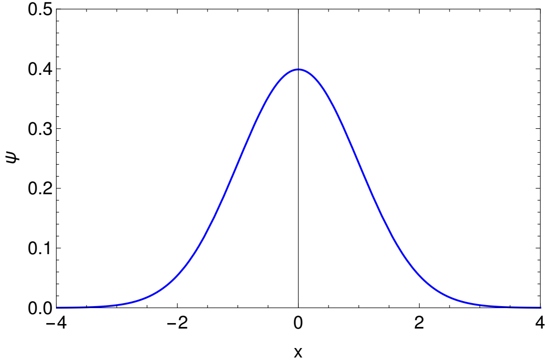
Getting the coefficients

$$b(k) = \langle \phi(k) | \psi \rangle \qquad P_n = |b(k)|^2$$

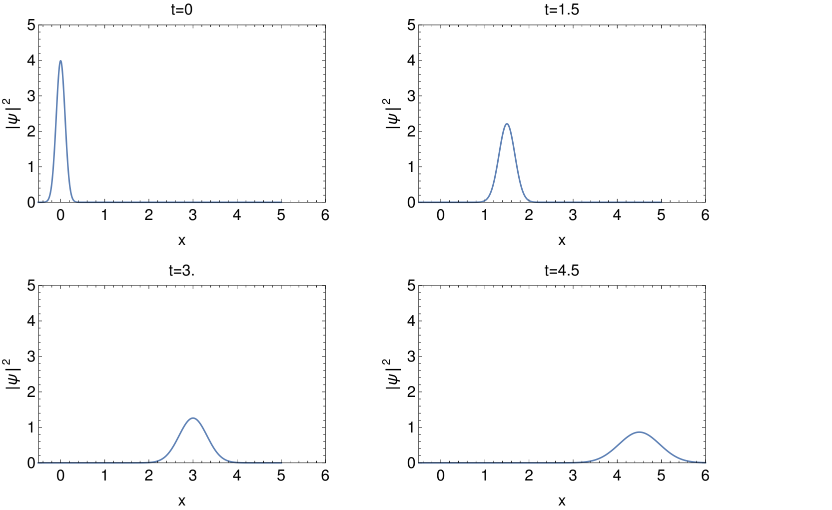
Time Development of the Initial Gaussian

Recall the Gaussian initial wave packet for the free particle shown below. How does it evolve in time?

$$V(x) = 0 \qquad |\Psi(x,0)\rangle = \frac{1}{(2\pi\sigma^2)^{1/4}} e^{-x^2/4\sigma^2}$$



Time Development of the Initial Gaussian



Time Development of Nuclear Fusion

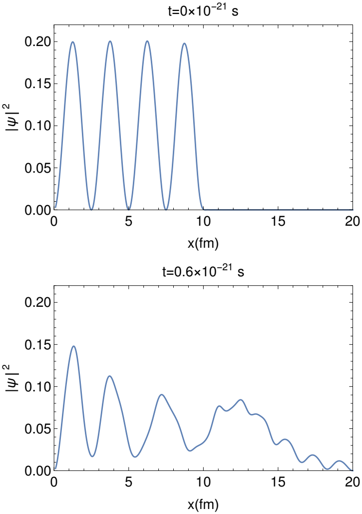
Consider a case of one dimensional nuclear 'fusion'. A neutron is in the potential well of a nucleus that we will approximate with an infinite square well with walls at $x = 0$ and $x = L$. The eigenfunctions and eigenvalues are

$$E_n = \frac{n^2\hbar^2\pi^2}{2ma^2} \qquad \begin{aligned} \phi_n &= \sqrt{\frac{2}{a}}\,\sin\left(\frac{n\pi x}{a}\right) & \quad 0 \leq x \leq a \\ &= 0 & \quad x < 0 \text{ and } x > a \end{aligned} \quad .$$

The neutron is in the $n = 4$ state when it fuses with another nucleus that is the same size, instantly putting the neutron in a new infinite square well with walls at $x = 0$ and $x = 2a$.

1. What are the new eigenfunctions and eigenvalues of the fused system?
2. How will the initial wave packet evolve in time?

Time Development of Nuclear Fusion



Comparison of Bound and Free Particles

Particle in a Box

The potential

$$V = 0 \qquad 0 < x < a$$
$$= \infty \qquad otherwise$$

Eigenfunctions and eigenvalues

$$|\phi_n\rangle = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \qquad E_n = n^2 \frac{\hbar^2 \pi^2}{2ma^2}$$

Superposition

$$|\psi\rangle = \sum_{n=1}^{\infty} b_n |\phi_n\rangle \qquad \langle \phi_m | \phi_n \rangle = \delta_{m,n}$$

Getting the coefficients

$$b_n = \langle \phi_n | \psi \rangle \qquad P_n = |b_n|^2$$

Time Dependence

$$\Psi(x,t) = \sum_{n=1}^{\infty} b_n |\phi_n(x)\rangle e^{-i\omega_n t}$$

Free Particle

The potential

$$V = 0$$

Eigenfunctions and eigenvalues

$$|\phi(k)\rangle = \frac{1}{\sqrt{2\pi}} e^{\pm ikx} \qquad E = \frac{\hbar^2 k^2}{2m}$$

Superposition

$$|\psi\rangle = \int_{-\infty}^{\infty} b(k)\phi(k) dk$$
$$\langle \phi(k') | \phi(k) \rangle = \delta(k - k')$$

Getting the coefficients

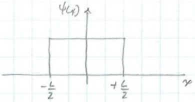
$$b(k) = \langle \phi(k) | \psi \rangle \qquad P_n = |b(k)|^2$$

Time Dependence

$$\Psi(x,t) = \int_{-\infty}^{\infty} b(k)\phi_k(x) e^{-i\omega(k)t} dk$$

Liboff 6.4 -

6.4 $N = 10^5$ protons $L = 10\,\text{cm}$



$$|\psi(x,0)\rangle = \frac{1}{\sqrt{L}} \qquad |x| \le L/2$$
$$= 0 \qquad \text{elsewhere}$$

$$\text{answer} = ? = \int_{-L/2}^{L/2} |\psi(x, t = 10\,s)|^2 \, dx$$

$$|\psi(x,0)\rangle = \int_{-\infty}^{+\infty} b(k)\, \phi(k)\, dk$$

$$\phi = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

$$b(k) = \langle \phi(k) | \psi \rangle$$
$$= \int_{-L/2}^{L/2} \frac{1}{\sqrt{2\pi}} e^{-ikx} \frac{1}{\sqrt{L}} \, dx$$
$$= \frac{1}{\sqrt{2\pi L}} \int_{-L/2}^{L/2} e^{-ikx} \, dx$$
$$= \frac{1}{\sqrt{2\pi L}} \frac{e^{-ikL/2} - e^{+ikL/2}}{-ik}$$
$$= \frac{1}{\sqrt{2\pi L}} \frac{e^{ikL/2} - e^{-ikL/2}}{i} \frac{1}{k}$$
$$= \frac{1}{\sqrt{2\pi L}} \frac{2 \sin kL/2}{k} \frac{L/2}{L/2}$$
$$= \sqrt{\frac{L}{2\pi}} \frac{\sin kL/2}{kL/2}$$

using the hint

$$|\psi(x,t)|^2 = \frac{1}{2\pi}\int\int_{-\infty}^{+\infty} b^*(k')\, b(k)\, e^{-ik'x}\, e^{i\omega' t} \times e^{ikx}\, e^{-i\omega t}\, dk'\, dk$$

$$= \frac{1}{2\pi}\int\int_{-\infty}^{+\infty} \left(\frac{L}{2\pi}\right) \frac{\sin k'L/2}{k'L/2}\, \frac{\sin kL/2}{kL/2} \times e^{i(k-k')x}\, e^{i(\omega'-\omega)t}\, dk'\, dk$$

$$\omega = \frac{\hbar k^2}{2m}$$

$$= \frac{L}{4\pi^2}\int\int_{-\infty}^{+\infty} \frac{\sin k'L/2}{k'L/2}\, \frac{\sin kL/2}{kL/2} \times e^{i(k-k')x}\, e^{i\hbar(k'^2-k^2)/2m}\, dk'\, dk$$

$$= \frac{L}{4\pi^2}\int_{-\infty}^{+\infty} \frac{\sin kL/2}{kL/2}\, e^{ikx}\, e^{-i\hbar k^2/2m} \times \int_{-\infty}^{+\infty} \frac{\sin k'L/2}{k'L/2}\, e^{-ik'x}\, e^{i\hbar k'^2/2m}\, dk'\, dk$$

Mathematica result

$$\int_{-\infty}^{\infty} \frac{\text{Sin}\left[\frac{k*L0}{2}\right]}{\frac{k*L0}{2}} * \text{Exp}[-i*k*x]*\text{Exp}\left[\frac{i*\text{hbar}*k^2*t}{2*\text{mp}}\right] dk$$

$$\text{ConditionalExpression}\Bigg[\frac{1}{48\, L0 \left(\frac{\text{hbar}^2 t^2}{\text{mp}^2}\right)^{5/4}}$$

$$\sqrt{\pi}\Bigg(\frac{1}{\text{mp}} i\, \text{hbar}\, t \Bigg(24 \sqrt{\frac{\text{hbar}^2 t^2}{\text{mp}^2}} (L0-2x)\, \text{HypergeometricPFQ}\left[\left\{\frac{1}{4}\right\}, \left\{\frac{1}{2}, \frac{5}{4}\right\}, -\frac{\text{mp}^2 (L0-2x)^4}{256\, \text{hbar}^2 t^2}\right] + 24 \sqrt{\frac{\text{hbar}^2 t^2}{\text{mp}^2}} (L0+2x)\, \text{HypergeometricPFQ}\left[\left\{\frac{1}{4}\right\}, \left\{\frac{1}{2}, \frac{5}{4}\right\},\right.$$

$$\left. -\frac{\text{mp}^2 (L0+2x)^4}{256\, \text{hbar}^2 t^2}\right] - (L0-2x)^3\, \text{HypergeometricPFQ}\left[\left\{\frac{3}{4}\right\}, \left\{\frac{3}{2}, \frac{7}{4}\right\}, -\frac{\text{mp}^2 (L0-2x)^4}{256\, \text{hbar}^2 t^2}\right] - (L0+2x)^3\, \text{HypergeometricPFQ}\left[\left\{\frac{3}{4}\right\}, \left\{\frac{3}{2}, \frac{7}{4}\right\}, -\frac{\text{mp}^2 (L0+2x)^4}{256\, \text{hbar}^2 t^2}\right]\Bigg) +$$

$$\sqrt{\frac{\text{hbar}^2 t^2}{\text{mp}^2}} \Bigg(24 \sqrt{\frac{\text{hbar}^2 t^2}{\text{mp}^2}} (L0-2x)\, \text{HypergeometricPFQ}\left[\left\{\frac{1}{4}\right\}, \left\{\frac{1}{2}, \frac{5}{4}\right\}, -\frac{\text{mp}^2 (L0-2x)^4}{256\, \text{hbar}^2 t^2}\right] + 24 \sqrt{\frac{\text{hbar}^2 t^2}{\text{mp}^2}} (L0+2x)\, \text{HypergeometricPFQ}\left[\left\{\frac{1}{4}\right\},\right.$$

$$\left.\left\{\frac{1}{2}, \frac{5}{4}\right\}, -\frac{\text{mp}^2 (L0+2x)^4}{256\, \text{hbar}^2 t^2}\right] + (L0-2x)^3\, \text{HypergeometricPFQ}\left[\left\{\frac{3}{4}\right\}, \left\{\frac{3}{2}, \frac{7}{4}\right\}, -\frac{\text{mp}^2 (L0-2x)^4}{256\, \text{hbar}^2 t^2}\right] + (L0+2x)^3\, \text{HypergeometricPFQ}\left[\left\{\frac{3}{4}\right\}, \left\{\frac{3}{2}, \frac{7}{4}\right\}, -\frac{\text{mp}^2 (L0+2x)^4}{256\, \text{hbar}^2 t^2}\right]\Bigg)\Bigg),$$

$$\frac{\text{hbar}\, t}{\text{mp}} \in \mathbb{R}\ \&\&\ \text{Im}[L0] + 2\, \text{Im}[x] \le 0\ \&\&\ \Big(\big(L0 \in \mathbb{R}\ \&\&\ x \in \mathbb{R}\ \&\&\ \big((L0\ |\ x) \in \mathbb{R}\ ||\ \text{Im}[L0] < 0\ ||\ (\text{Im}[x] < 0\ \&\&\ \text{Im}[L0] \le 2\, \text{Im}[x])\ ||\ \text{Im}[x] > 0\big)\big)\ ||\ (\text{Im}[L0] < 0\ \&\&\ \text{Im}[L0] \le 2\, \text{Im}[x])\Big)\Bigg]$$

Mathematica result

$$\text{Assuming}\Big[k \in \text{Reals} \;\&\&\; L0 \in \text{Reals} \;\&\&\; L0 > 0 \;\&\&\; \text{hbar} \in \text{Reals} \;\&\&\; \text{hbar} > 0 \;\&\&\; \text{mp} \in \text{Reals} \;\&\&\; \text{mp} > 0 \;\&\&\; t \in \text{Reals} \;\&\&\; t > 0 \;\&\&\; x \in \text{Reals},$$

$$\int_{-\infty}^{\infty} \frac{\text{Sin}\left[\frac{k*L0}{2}\right]}{\frac{k*L0}{2}} * \text{Exp}[-i*k*x] * \text{Exp}\left[\frac{i*\text{hbar}*k^2*t}{2*\text{mp}}\right] dk\Big]$$

$$\frac{1}{48\, L0\, (\text{hbar}\, t)^{3/2}} \sqrt{\text{mp}}\, \sqrt{\pi} \Bigg(24\, \text{hbar}\, t\, (L0 - 2x)\, \text{HypergeometricPFQ}\left[\left\{\frac{1}{4}\right\}, \left\{\frac{1}{2}, \frac{5}{4}\right\}, -\frac{\text{mp}^2 (L0 - 2x)^4}{256\, \text{hbar}^2\, t^2}\right] +$$

$$24\, \text{hbar}\, t\, (L0 + 2x)\, \text{HypergeometricPFQ}\left[\left\{\frac{1}{4}\right\}, \left\{\frac{1}{2}, \frac{5}{4}\right\}, -\frac{\text{mp}^2 (L0 + 2x)^4}{256\, \text{hbar}^2\, t^2}\right] + \text{mp}\, (L0 - 2x)^3\, \text{HypergeometricPFQ}\left[\left\{\frac{3}{4}\right\}, \left\{\frac{3}{2}, \frac{7}{4}\right\}, -\frac{\text{mp}^2 (L0 - 2x)^4}{256\, \text{hbar}^2\, t^2}\right] +$$

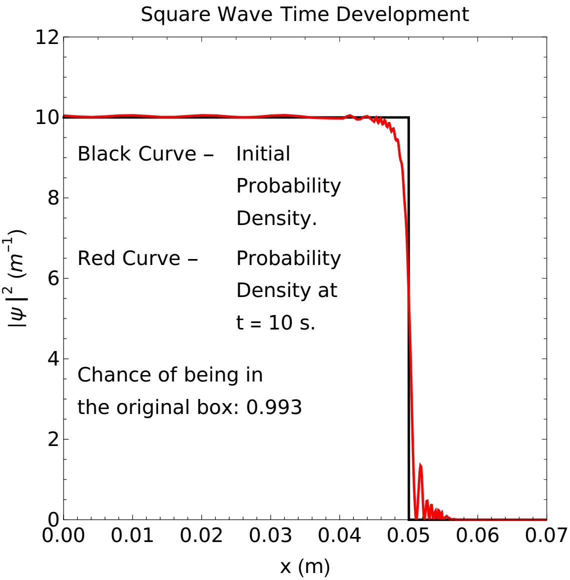
$$\text{mp}\, (L0 + 2x)^3\, \text{HypergeometricPFQ}\left[\left\{\frac{3}{4}\right\}, \left\{\frac{3}{2}, \frac{7}{4}\right\}, -\frac{\text{mp}^2 (L0 + 2x)^4}{256\, \text{hbar}^2\, t^2}\right] - \frac{1}{\text{Abs}\left[L0^2 - 4x^2\right]}$$

$$i\, \text{Abs}[L0 - 2x]\, \text{Abs}[L0 + 2x] \Bigg(-24\, \text{hbar}\, t\, (L0 - 2x)\, \text{HypergeometricPFQ}\left[\left\{\frac{1}{4}\right\}, \left\{\frac{1}{2}, \frac{5}{4}\right\}, -\frac{\text{mp}^2 (L0 - 2x)^4}{256\, \text{hbar}^2\, t^2}\right] -$$

$$24\, \text{hbar}\, t\, (L0 + 2x)\, \text{HypergeometricPFQ}\left[\left\{\frac{1}{4}\right\}, \left\{\frac{1}{2}, \frac{5}{4}\right\}, -\frac{\text{mp}^2 (L0 + 2x)^4}{256\, \text{hbar}^2\, t^2}\right] +$$

$$\text{mp} \left((L0 - 2x)^3\, \text{HypergeometricPFQ}\left[\left\{\frac{3}{4}\right\}, \left\{\frac{3}{2}, \frac{7}{4}\right\}, -\frac{\text{mp}^2 (L0 - 2x)^4}{256\, \text{hbar}^2\, t^2}\right] + (L0 + 2x)^3\, \text{HypergeometricPFQ}\left[\left\{\frac{3}{4}\right\}, \left\{\frac{3}{2}, \frac{7}{4}\right\}, -\frac{\text{mp}^2 (L0 + 2x)^4}{256\, \text{hbar}^2\, t^2}\right]\right)\Bigg)\Bigg)$$

Liboff 6.4 - 5



Square Wave Time Development
12
10
8
6
4
2
0
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07
x (m)
$|\psi|^2\ (m^{-1})$
Black Curve – Initial Probability Density.
Red Curve – Probability Density at t = 10 s.
Chance of being in the original box: 0.993