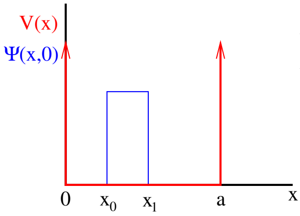
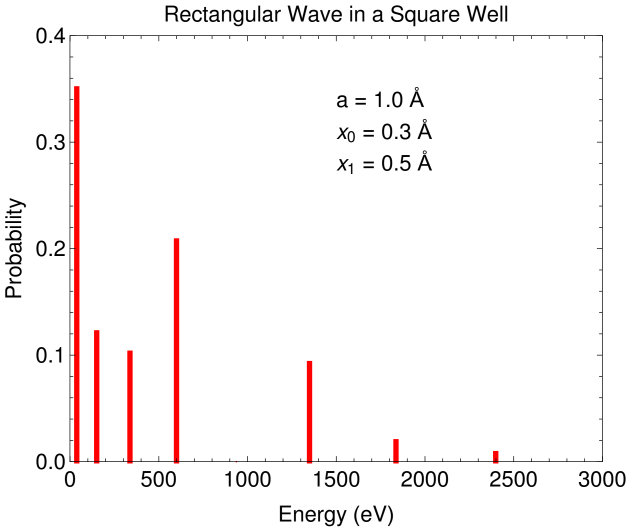
Recall the rectangular initial wave packet in the infinite square well shown below. How does it evolve in time?

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

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

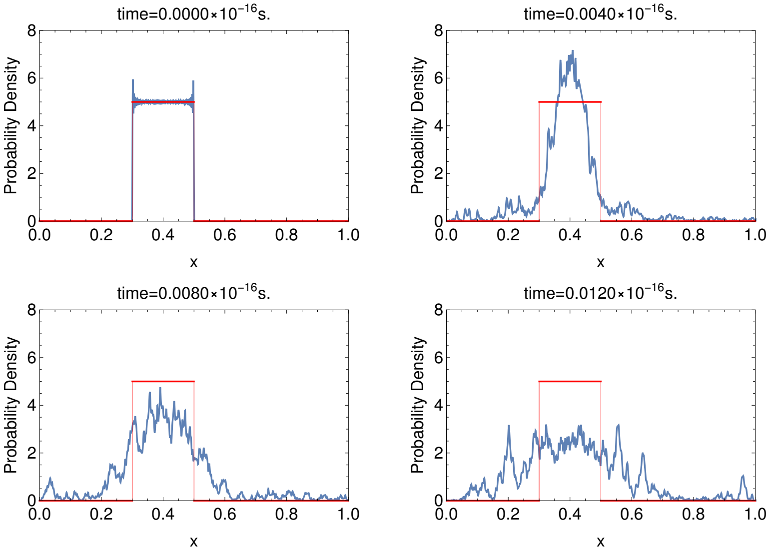


$$a = 1.0 \text{ Å}$$
$$x_0 = 0.3 \text{ Å}$$
$$x_1 = 0.5 \text{ Å}$$



Rectangular Wave in a Square Well
a = 1.0 Å
x_0 = 0.3 Å
x_1 = 0.5 Å
Probability
0.0
0.1
0.2
0.3
0.4
0
500
1000
1500
2000
2500
3000
Energy (eV)

Time Development of a Square Wave 3



Particle in a Box

The potential

$$V = 0 \qquad 0 < x < a$$
$$= \infty \qquad \textit{otherwise}$$

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

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

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

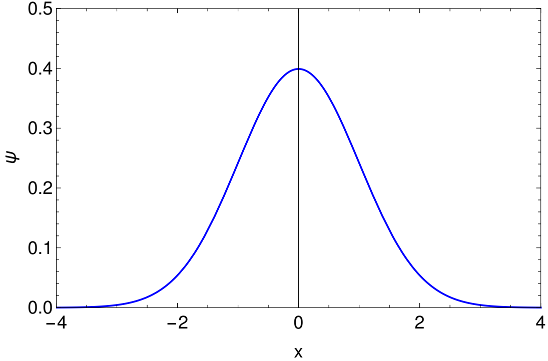
$$|\psi\rangle = \int_{-\infty}^{\infty} b(k)\phi(k)dk$$
$$\langle \phi(k') | \phi(k) \rangle = \delta(k - k')$$

Getting the coefficients

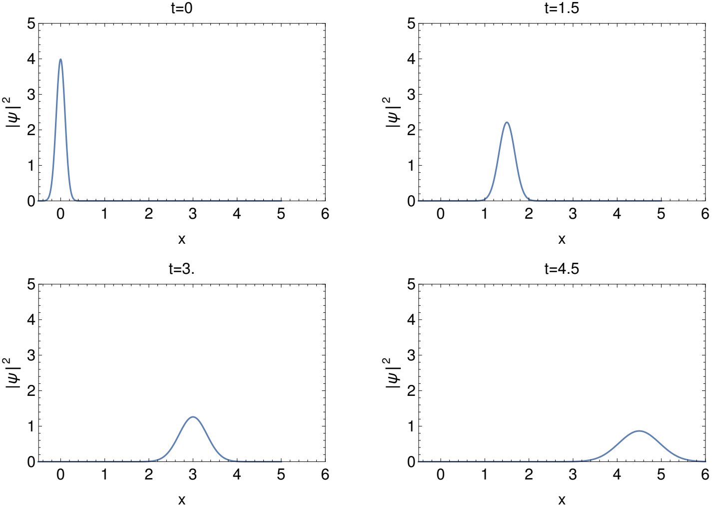
$$b(k) = \langle \phi(k) | \psi \rangle \qquad P_n = |b(k)|^2$$

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 6

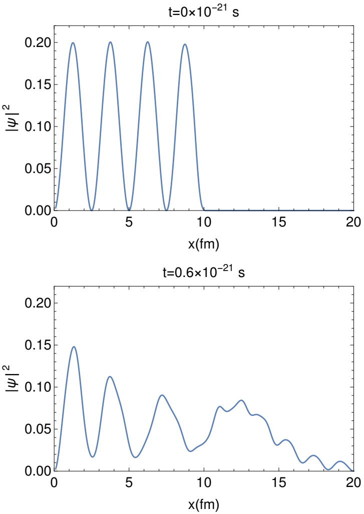


Consider a case of one dimensional nuclear 'fusion'. A neutron is in the potential well of a nucleus that we will approximate with an infinite square well with walls at $x = 0$ and $x = L$. The eigenfunctions and eigenvalues are

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

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?



t=0×10^-21 s
t=0.3×10^-21 s
t=0.6×10^-21 s
t=0.9×10^-21 s
|ψ|^2
x(fm)
0.00
0.05
0.10
0.15
0.20
0
5
10
15
20

Particle in a Box

The potential

$$V = 0 \qquad 0 < x < a$$
$$= \infty \qquad \textit{otherwise}$$

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

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

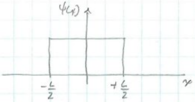
Getting the coefficients

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

Time Dependence

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

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



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

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

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

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

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

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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

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

$$\begin{aligned}
&\text{ConditionalExpression}\Bigg[\frac{1}{48\ \text{L0}\left(\frac{\text{hbar}^2\ t^2}{\text{mp}^2}\right)^{5/4}} \\
&\sqrt{\pi}\left(\frac{1}{\text{mp}} i\ \text{hbar}\ t\left(24\sqrt{\frac{\text{hbar}^2\ t^2}{\text{mp}^2}}\ (\text{L0}-2\ x)\ \text{HypergeometricPFQ}\left[\left\{\frac{1}{4}\right\},\left\{\frac{1}{2},\frac{5}{4}\right\},-\frac{\text{mp}^2\ (\text{L0}-2\ x)^4}{256\ \text{hbar}^2\ t^2}\right]+24\sqrt{\frac{\text{hbar}^2\ t^2}{\text{mp}^2}}\ (\text{L0}+2\ x)\ \text{HypergeometricPFQ}\left[\left\{\frac{1}{4}\right\},\left\{\frac{1}{2},\frac{5}{4}\right\},\right.\right.\right. \\
&\quad \left.-\frac{\text{mp}^2\ (\text{L0}+2\ x)^4}{256\ \text{hbar}^2\ t^2}\right]-(\text{L0}-2\ x)^3\ \text{HypergeometricPFQ}\left[\left\{\frac{3}{4}\right\},\left\{\frac{3}{2},\frac{7}{4}\right\},-\frac{\text{mp}^2\ (\text{L0}-2\ x)^4}{256\ \text{hbar}^2\ t^2}\right]-(\text{L0}+2\ x)^3\ \text{HypergeometricPFQ}\left[\left\{\frac{3}{4}\right\},\left\{\frac{3}{2},\frac{7}{4}\right\},-\frac{\text{mp}^2\ (\text{L0}+2\ x)^4}{256\ \text{hbar}^2\ t^2}\right]\Bigg)+ \\
&\sqrt{\frac{\text{hbar}^2\ t^2}{\text{mp}^2}}\left(24\sqrt{\frac{\text{hbar}^2\ t^2}{\text{mp}^2}}\ (\text{L0}-2\ x)\ \text{HypergeometricPFQ}\left[\left\{\frac{1}{4}\right\},\left\{\frac{1}{2},\frac{5}{4}\right\},-\frac{\text{mp}^2\ (\text{L0}-2\ x)^4}{256\ \text{hbar}^2\ t^2}\right]+24\sqrt{\frac{\text{hbar}^2\ t^2}{\text{mp}^2}}\ (\text{L0}+2\ x)\ \text{HypergeometricPFQ}\left[\left\{\frac{1}{4}\right\},\right.\right. \\
&\quad \left.\left\{\frac{1}{2},\frac{5}{4}\right\},-\frac{\text{mp}^2\ (\text{L0}+2\ x)^4}{256\ \text{hbar}^2\ t^2}\right]+(\text{L0}-2\ x)^3\ \text{HypergeometricPFQ}\left[\left\{\frac{3}{4}\right\},\left\{\frac{3}{2},\frac{7}{4}\right\},-\frac{\text{mp}^2\ (\text{L0}-2\ x)^4}{256\ \text{hbar}^2\ t^2}\right]+(\text{L0}+2\ x)^3\ \text{HypergeometricPFQ}\left[\left\{\frac{3}{4}\right\},\left\{\frac{3}{2},\frac{7}{4}\right\},-\frac{\text{mp}^2\ (\text{L0}+2\ x)^4}{256\ \text{hbar}^2\ t^2}\right]\Bigg)\Bigg), \\
&\frac{\text{hbar}\ t}{\text{mp}} \in \mathbb{R}\ \&\&\ \text{Im}[\text{L0}]+2\ \text{Im}[x] \le 0\ \&\&\ \Big(\big(\text{L0} \in \mathbb{R}\ \&\&\ x \in \mathbb{R}\ \&\&\ \big((\text{L0}\ |\ x) \in \mathbb{R}\ ||\ \text{Im}[\text{L0}] < 0\ ||\ (\text{Im}[x] < 0\ \&\&\ \text{Im}[\text{L0}] \le 2\ \text{Im}[x])\ ||\ \text{Im}[x] > 0\big)\big)\ ||\ (\text{Im}[\text{L0}] < 0\ \&\&\ \text{Im}[\text{L0}] \le 2\ \text{Im}[x])\Big)\Bigg]
\end{aligned}$$

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Mathematica result

```
Assuming[k ∈ Reals && L0 ∈ Reals && L0 > 0 && hbar ∈ Reals && hbar > 0 && mp ∈ Reals && mp > 0 && t ∈ Reals && t > 0 && x ∈ Reals ,
 ∫_{-∞}^{∞} Sin[k*L0/2]/(k*L0/2) * Exp[-i*k*x] * Exp[(i*hbar*k^2*t)/(2*mp)] dk]
```

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

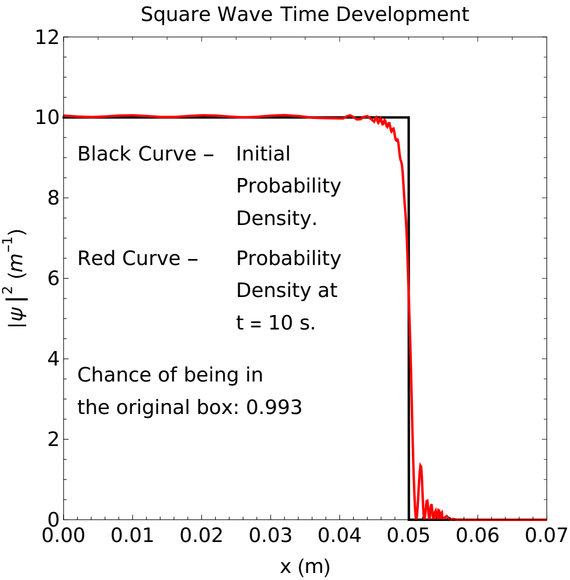
$$24\ \text{hbar t}\ (\text{L0}+2\ \text{x})\ \text{HypergeometricPFQ}\left[\left\{\frac{1}{4}\right\},\left\{\frac{1}{2},\frac{5}{4}\right\},-\frac{\text{mp}^2\ (\text{L0}+2\ \text{x})^4}{256\ \text{hbar}^2\ \text{t}^2}\right]+\text{mp}\ (\text{L0}-2\ \text{x})^3\ \text{HypergeometricPFQ}\left[\left\{\frac{3}{4}\right\},\left\{\frac{3}{2},\frac{7}{4}\right\},-\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

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

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

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

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


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