1. Solve the Schroedinger equation to get eigenfunctions and eigenvalues.

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi(x)}{\partial x^2} + V\phi(x) = E\phi(x)$$

2. For an initial wave packet $\psi(x)$ use the completeness of the eigenfunctions.

$$|\psi(x)\rangle = \sum_{n=1}^{\infty} b_n|\phi(x)\rangle$$

3. Apply the orthonormality $\langle\phi_m|\phi_n\rangle = \delta_{m,n}$.

$$\langle\phi_m|\psi\rangle = \langle\phi_m|\left(\sum_{n=1}^{\infty} b_n|\phi\rangle\right) = b_m = \int_{-\infty}^{\infty} \phi_m^* \left(\sum_{n=1}^{\infty} b_n|\phi\rangle\right) dx$$

4. Get the probability P_n for measuring E_n from $|\psi\rangle$. of $|\psi\rangle$.

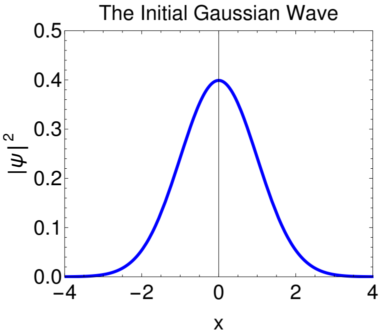
$$P_n = |b_n|^2$$

5. Do the free particle solution.
6. Put in the time evolution.

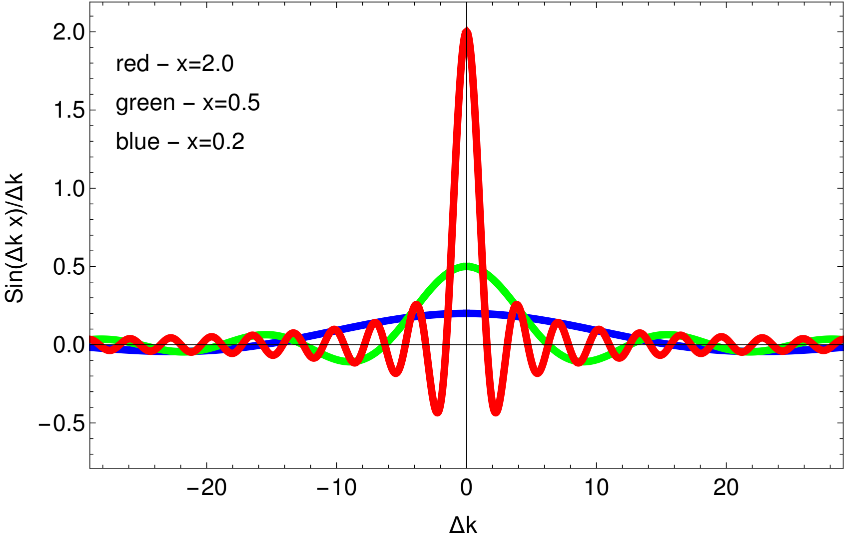
Consider a free particle ($V = 0$) which has an initial wave packet that is described by a gaussian function.

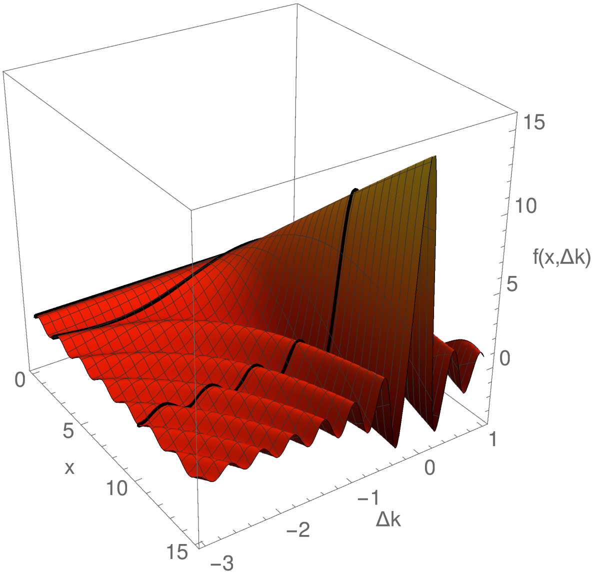
$$|\Psi(x,0)\rangle = \frac{1}{(2\pi\sigma^2)^{1/4}} e^{-x^2/4\sigma^2}$$

What is the spectrum of momenta that form this wave packet? How wide is that distribution?

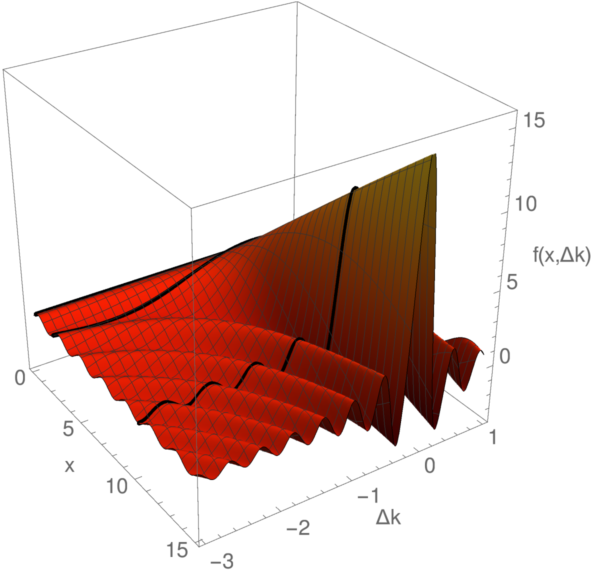


3


red – x=2.0
green – x=0.5
blue – x=0.2
Sin(Δk x)/Δk
Δk
2.0
1.5
1.0
0.5
0.0
−0.5
−20
−10
0
10
20

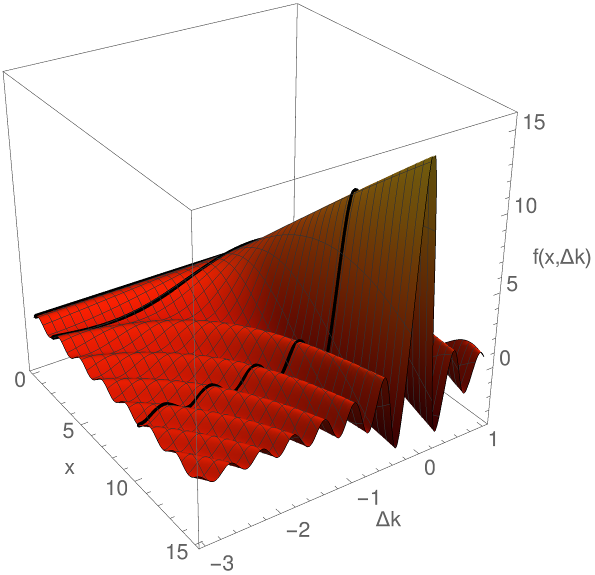


15
10
f(x,Δk)
5
0
0
5
x
10
15
1
0
−1
Δk
−2
−3



$$\int_{-\Delta k_{max}}^{\Delta k_{max}} \lim_{x \to \infty} \frac{\sin(\Delta k\, x)}{\Delta k} d(\Delta k)$$

x	Δk_{max}	Integral
0.01	10000	3.12445
1.0	10000	3.14178
2.0	10000	3.14151
4.0	10000	3.14158
10.0	10000	3.14161
100.0	10000	3.14159
1000.0	10000	3.14159
10000.0	10000	3.14159
100000.0	10000	3.14159



$$\int_{-\Delta k_{max}}^{\Delta k_{max}} \lim_{x \to \infty} \frac{\sin(\Delta k\, x)}{\Delta k} d(\Delta k)$$

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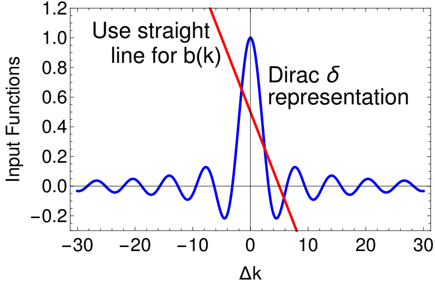
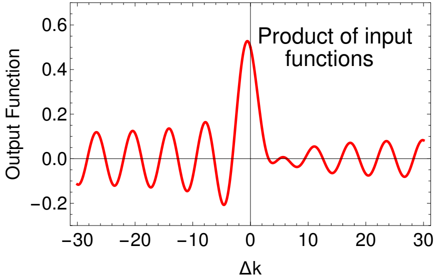
1000.0	10000	3.14159
10000.0	10000	3.14159
100000.0	10000	3.14159

Dirac Delta Function Demonstration 7





$$\int_{-\Delta k_{max}}^{\Delta k_{max}} 2b(k) \lim_{x \to \infty} \frac{\sin(\Delta k\, x)}{\Delta k} d(\Delta k) =$$

$$2b(k') \int_{-\Delta k_{max}}^{\Delta k_{max}} \lim_{x \to \infty} \frac{\sin(\Delta k\, x)}{\Delta k} d(\Delta k)$$

$$2b(k=0) = 1.0$$

x on $l.h.s.$	Δk_{max}	$l.h.s$	$r.h.s$
0.01	1000	3.31670	3.14159
1.0	1000	3.14047	3.14159
2.0	1000	3.14196	3.14159
10.0	1000	3.14178	3.14159
100.0	1000	3.14161	3.14159
1000.0	1000	3.14159	3.14159
10000.0	1000	3.14159	3.14159
100000.0	1000	3.14159	3.14159

Particle in a Box

The potential

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

Eigenfunctions and eigenvalues

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

Superposition

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

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

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

Superposition

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

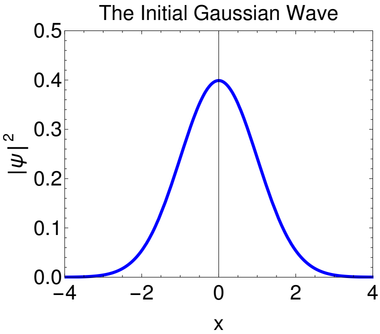
Getting the coefficients

$$b(k) = \langle \phi(k) | \psi \rangle \quad P(k)dk = |b(k)|^2 dk$$

Consider a free particle ($V = 0$) which has an initial wave packet that is described by a gaussian function.

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

What is the spectrum of momenta that form this wave packet? How wide is that distribution?



(3.37) $$\psi(x, t) = A \exp\left[\frac{-(x - x_0)^2}{4a^2}\right] \exp\left(\frac{ip_0 x}{\hbar}\right) \exp(i\omega_0 t)$$

3.10 For the state ψ, given by (3.37), show that

$$(\Delta x)^2 = a^2$$

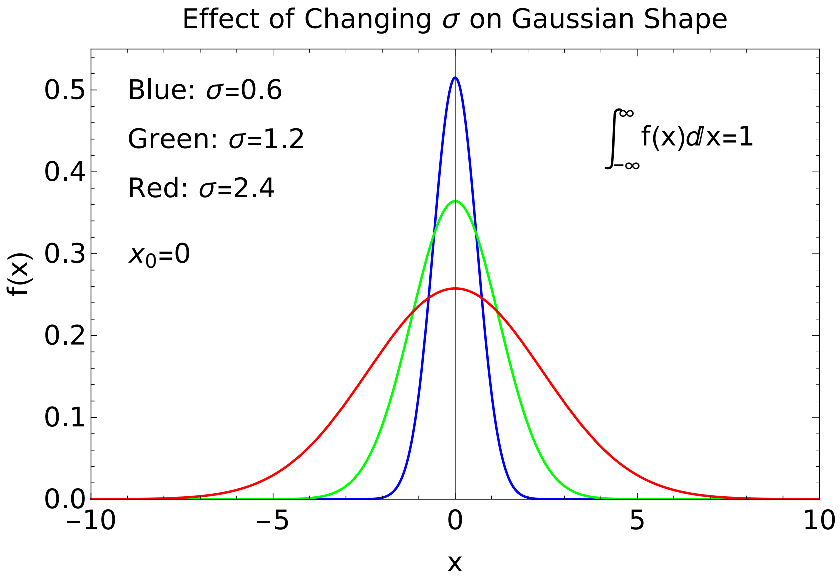
Argue the consistency of this conclusion with the change in shape that $|\psi|^2$ suffers with a change in the parameter a.

In the solution to 3.10

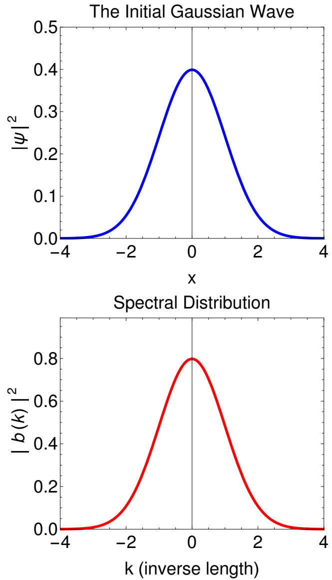
$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 \quad \text{and} \quad \langle x^2 \rangle = a^2 + x_0^2 \quad \text{and} \quad \langle x \rangle^2 = x_0^2$$

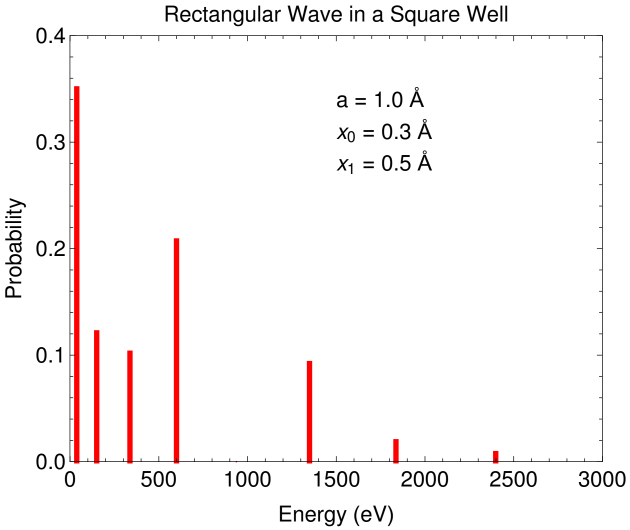
so

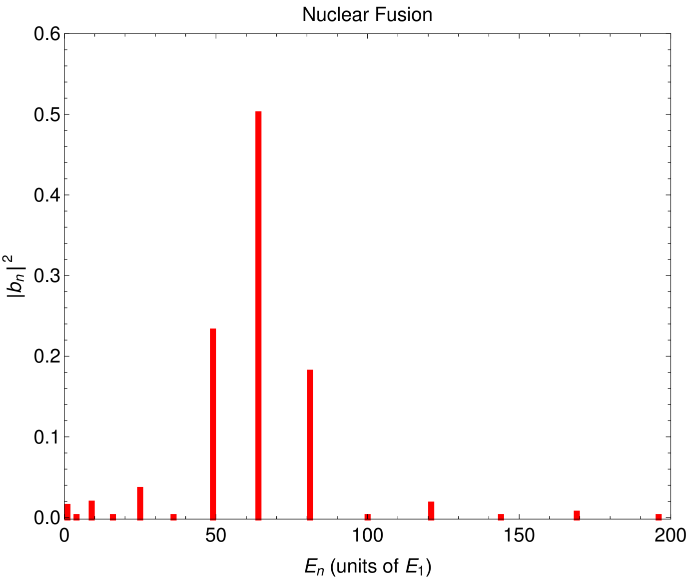
$$(\Delta x)^2 = a^2 + x_0^2 - x_0^2 = a^2$$

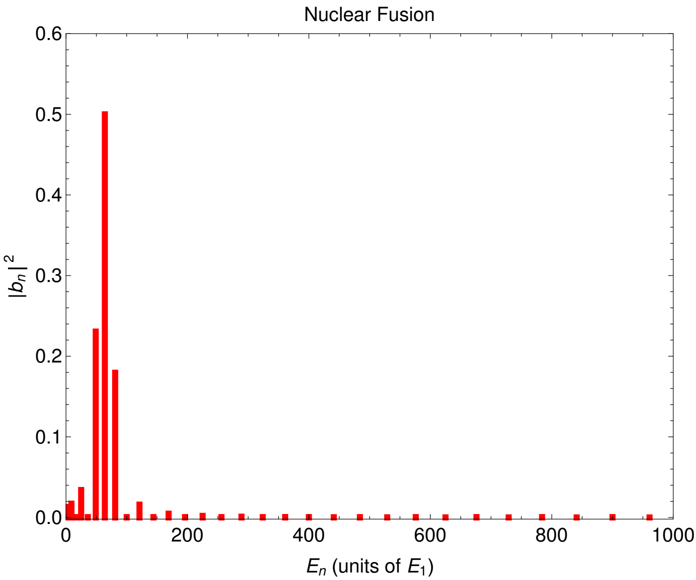


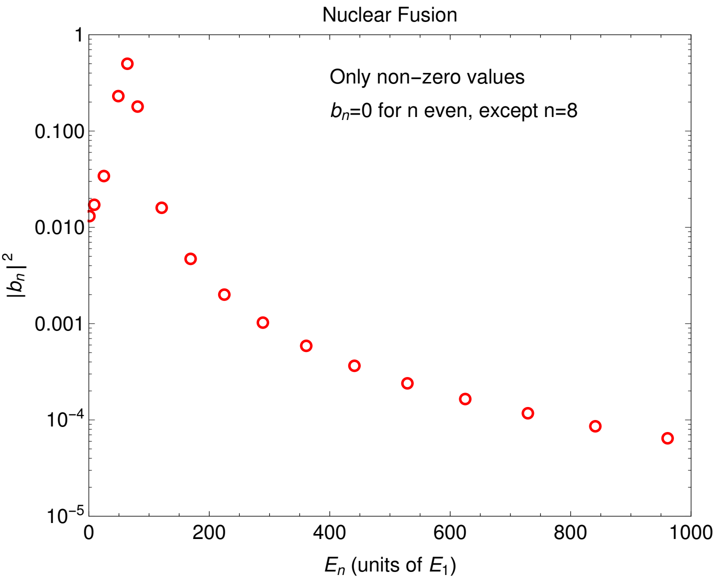
Effect of Changing σ on Gaussian Shape
Blue: σ=0.6
Green: σ=1.2
Red: σ=2.4
x_0=0
$\int_{-\infty}^{\infty} f(x)dx=1$
f(x)
x
0.5
0.4
0.3
0.2
0.1
0.0
−10
−5
0
5
10


The Initial Gaussian Wave
0.5
0.4
0.3
0.2
0.1
0.0
|ψ|²
−4
−2
0
2
4
x
Spectral Distribution
0.8
0.6
0.4
0.2
0.0
| b(k) |²
−4
−2
0
2
4
k (inverse length)


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)


Nuclear Fusion
0.6
0.5
0.4
0.3
0.2
0.1
0.0
$|b_n|^2$
0
50
100
150
200
E_n (units of E_1)


Nuclear Fusion
0.6
0.5
0.4
0.3
0.2
0.1
0.0
$|b_n|^2$
0
200
400
600
800
1000
E_n (units of E_1)


Nuclear Fusion
Only non−zero values
b_n=0 for n even, except n=8
1
0.100
0.010
0.001
10^{-4}
10^{-5}
$|b_n|^2$
0
200
400
600
800
1000
E_n (units of E_1)