$\vec{S} = \mathrm{Re}\left[\psi^* \frac{\hbar\vec{\nabla}}{im}\psi\right]$

1.3.2. Free Particle Wave Functions

a. Plane Waves

The free particle, $V=0$ (or constant), Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t)$$

has, as stated earlier, the plane wave solutions

$$\psi_{\vec{k}}(\vec{r},t) = \frac{1}{N}e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

with N a normalization constant and ω and $\vec{k}$ related by $\hbar\omega = \frac{\hbar^2\vec{k}^2}{2m}$.

Note that $\vec{k}$ is unrestricted, it can take on a 3-fold continuum of values. Since this is a particle of single frequency we can identify the energy as $E=\hbar\omega$ according to the Planck-Einstein relation and the momentum as $\vec{p}=\hbar\vec{k}$ by deBroglie's hypothesis.

Thus we have that $E=\frac{\vec{p}^2}{2m}$, the energy-momentum relation for a single free particle as we know from classical mechanics.

Since $|\psi_{\vec{k}}|^2 = |N|^2$ is a constant, the plane wave has a uniform position probability density everywhere in space. Such a particle is completely unlocalized in space: it has the same probability to be anywhere. Consequently the plane wave wavefunction is not square integrable (not normalizable) and therefore cannot correspond to a physically realizable state of the system. As we will see, it is often convenient to use plane wave states for mathematical simplicity; if a question of rigor arises we can instead use normalizable solutions to Schrödinger's equation for intermediate steps and at the end take the plane wave limit. As can be shown, there is no ambiguity in such a procedure.

In fact there are many ways to handle this situation. One simple way to make the plane wave solutions normalizable is to place the system in a box of finite spatial extent, say a cube with sides of length L, and so volume $V = L^3$. The finite volume of space will make the integrals convergent. At the end of the calculation of any physical observable the volume will be taken to infinity. Inside the box the solution to Schrödinger's equation will be (linear combinations) of plane waves

$$\psi_{\vec{k}}(\vec{r},t) = \frac{1}{N} e^{+i(\vec{k}\cdot\vec{r} - \omega t)}, \text{ where,}$$

to satisfy the Schrödinger equation,

$\hbar\omega = \frac{\hbar^2 \vec{k}^2}{2m}$. This is inside the box, we must now also specify the wave function on the surface of the box. Since at the end of the calculation of any physical observable the volume of the box will be taken to infinity, the precise form of the boundary condition will be physically irrelevant. No observable can depend on the volume or the choice of boundary condition on the surface of the box. Typically there are two common choices for the box boundary conditions:

1) The wavefunction vanishes on the surface of the box. This can be viewed physically as an infinite potential barrier occuring at the walls of the box. Such a situation will be investigated when we study a particle in a potential well.

2) Periodic boundary conditions so that

$$\psi_{\vec{k}}(x,y,z,t) = \psi_{\vec{k}}(x+L,y,z,t)$$
$$= \psi_{\vec{k}}(x,y+L,z,t)$$
$$= \psi_{\vec{k}}(x,y,z+L,t) .$$

The advantage of periodic boundary conditions will be to have wavefunctions that are also eigenfunctions of the Hermitian momentum operator $\vec{p} = -i\hbar\vec{\nabla}$.

Either choice of boundary condition, or any other choice for that matter, will lead to restrictions on the allowed values of $\vec{k}$. Consider the periodic boundary condition case with wavefunction

$$\psi_{\vec{k}}(\vec{r},t) = \frac{1}{N} e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

where $\hbar\omega = \frac{\hbar^2 k^2}{2m}$. The x-direction periodicity implies

$$e^{ik_x x} = e^{ik_x(x+L)},$$

this can be true only if $e^{ik_x L} = 1$ that is

$$k_x = \frac{2\pi}{L} n_x \quad , n_x = 0, \pm 1, \pm 2, \ldots .$$

Similarly the y and z periodicity conditions imply that

$$k_y = \frac{2\pi}{L} n_y \quad , n_y = 0, \pm 1, \pm 2, \ldots$$

$$k_z = \frac{2\pi}{L} n_z \quad , n_z = 0, \pm 1, \pm 2, \ldots .$$

Hence inside the box the wavefunction is

$$\psi_{\vec{k}}(\vec{r},t) = \psi_{n_x n_y n_z}(\vec{r},t)$$

$$= \frac{1}{N} e^{\frac{2\pi i}{L}(n_x x + n_y y + n_z z)} e^{-i\omega t}$$

with $n_x, n_y, n_z = 0, \pm 1, \pm 2, \pm 3, \ldots$ and

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2) .$$

By restricting the problem to finite volume the allowed $\vec{k}$ values (allowed solutions) no longer form a continuum but now only take on discrete values

$$(k_x, k_y, k_z) = \frac{2\pi}{L}(n_x, n_y, n_z), \quad n_{x,y,z} = 0, \pm 1, \pm 2, \ldots .$$

As $L \to \infty$, the boundary conditions are removed and the allowed $\vec{k}$ values again approach a continuum. The energy of the particle is now "quantized"

$$E = \hbar\omega = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

since $\vec{k}$ is "quantized" (has allowed discrete values). Besides $\psi_{n_x n_y n_z}$ being an eigenstate of energy,

$$H\psi_{n_x n_y n_z}(\vec{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi_{n_x n_y n_z}(\vec{r},t)$$
$$= E_{n_x n_y n_z}\psi_{n_x n_y n_z}(\vec{r},t),$$

it is also an eigenstate of the momentum operator

$$\vec{p}\,\psi_{n_x n_y n_z}(\vec{r},t) = -i\hbar\vec{\nabla}\psi_{n_x n_y n_z}(\vec{r},t)$$
$$= \hbar\vec{k}\,\psi_{n_x n_y n_z}(\vec{r},t)$$

with, as expected by the deBroglie relation, discrete momentum eigenvalues

$$\vec{p} = \hbar\vec{k} = \frac{2\pi\hbar}{L}(n_x, n_y, n_z).$$

Finally, since the wavefunction is restricted to inside the box it is square-integrable. In fact

$$\int_V d^3r\, \psi^*_{n_x' n_y' n_z'}(\vec{r},t)\,\psi_{n_x n_y n_z}(\vec{r},t)$$
$$= \frac{1}{|N|^2}\int_0^L dx\, e^{i\frac{2\pi}{L}(n_x - n_x')x} \times$$
$$\times \int_0^L dy\, e^{i\frac{2\pi}{L}(n_y - n_y')y} \int_0^L dz\, e^{i\frac{2\pi}{L}(n_z - n_z')z} \times$$
$$\times\, e^{-i(\omega(n_x,n_y,n_z) - \omega(n_x',n_y',n_z'))t}$$

Now if $n' \neq n$ then

$$\int_0^L dx\, e^{i\frac{2\pi}{L}(n-n')x} = \frac{1}{i\frac{2\pi}{L}(n-n')} \times \left[e^{i\frac{2\pi}{L}(n-n')L} - e^0 \right]$$

but $e^{i\frac{2\pi}{L}(n-n')L} = e^{i2\pi(n-n')} = 1 = e^0$

thus $\underline{\int_0^L dx\, e^{i\frac{2\pi}{L}(n-n')x} = 0 \text{ for } n' \neq n}$

For $n' = n$ we simply have

$$\int_0^L dx\, e^{i\frac{2\pi}{L}(n-n)x} = \int_0^L dx = L.$$

These can be summarized as

$$\int_0^L dx\, e^{i\frac{2\pi}{L}(n-n')x} = L\delta_{n'n}$$

where the Kronecker delta is given by

$$\delta_{n'n} = \begin{cases} 1 & \text{if } n' = n \\ 0 & \text{if } n' \neq n \end{cases}.$$

Thus we find

$$\int_V d^3r\, \psi^*_{n_x' n_y' n_z'}(\vec{r},t)\, \psi_{n_x n_y n_z}(\vec{r},t)$$

$$= \frac{1}{|N|^2} L^3 \delta_{n_x' n_x} \delta_{n_y' n_y} \delta_{n_z' n_z}$$

where the time phases cancel since the Kronecker deltas require $n'_{x,y,z} = n_{x,y,z}$ and hence $\omega(n_x', n_y', n_z') = \omega(n_x, n_y, n_z)$.

Since we are free to choose the normalization factor N at will, we may as well let

$$N = \sqrt{V} = L^{3/2}$$

so that the wavefunctions are orthonormal,

$$\psi_{n_x n_y n_z}(\vec{r},t) = \frac{1}{\sqrt{V}}\, e^{\frac{2\pi i}{L}(n_x x + n_y y + n_z z)}\, e^{-i\omega_{n_x n_y n_z} t}$$

with $\hbar\omega_{n_x n_y n_z} = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$.

Hence, the free particle wavefunctions become square-integrable once, we restrict the particle to finite volume, $0 \leq x \leq L$, $0 \leq y \leq L$, $0 \leq z \leq L$. This results in limiting the allowed values of the momentum to be discrete units of $\frac{2\pi\hbar}{L}$.

In practice we will continue to use plane wave wavefunctions. If interpretational difficulties should arise due to their non-square integrability, one can return to the finite volume wavefunctions and at the end of the calculation unambiguously let $V \to \infty$. As in the periodic boundary case, the plane wave wavefunctions are especially useful since they are eigenfunctions of the momentum operator. In fact since

$$-i\hbar\vec{\nabla}\,\psi_{\vec{k}}(\vec{r},t) = \hbar\vec{k}\,\psi_{\vec{k}}(\vec{r},t)$$

and by deBroglie's hypothesis, a monochromatic free particle wave function has momentum $\vec{p} = \hbar\vec{k}$, we are led to the identification of the momentum operator $\vec{p} = -i\hbar\vec{\nabla}$. This, as we argued with the probability current density is a valid identification even for a noninteracting particle.

1.3.2. Free Particle Wave Functions

b. Wave Packets

Alternatively, normalizable wave functions can be obtained by exploiting the principle of superposition. Since the Schrödinger equation is linear in $\psi(\vec{r},t)$, the sum of two solutions is also a solution to the equation. Hence we can add plane wave solutions with different wave vectors $\vec{k}$ to obtain a solution to the free Schrödinger equation. In fact mathematically it can be shown that every square integrable function can be written as a superposition of plane waves, this is the Fourier expansion theorem. Thus the most general solution to the free Schrödinger equation is given by

$$\psi(\vec{r},t) = \int \frac{d^3k}{(2\pi)^3}\, g(\vec{k})\, e^{i(\vec{k}\cdot\vec{r} - \omega_k t)}$$

where $\hbar\omega_k = \frac{\hbar^2 \vec{k}^2}{2m}$. The coefficient function $g(\vec{k})$, can be found by inverting the Fourier transform. Indeed, at $t=0$ we have

$$\psi(\vec{r},0) = \int \frac{d^3k}{(2\pi)^3}\, g(\vec{k})\, e^{i\vec{k}\cdot\vec{r}}.$$

Multiplying by $e^{-i\vec{k}'\cdot\vec{r}}$ and integrating over space yields

$$\int d^3r\, e^{-i\vec{k}'\cdot\vec{r}}\, \psi(\vec{r},0) = \int d^3r \frac{d^3k}{(2\pi)^3}\, g(\vec{k})\, e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}.$$

But the Fourier expansion of the Dirac delta function is just

$$\delta^3(\vec{k}-\vec{k}') = \int \frac{d^3r}{(2\pi)^3}\, e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}.$$

Thus we secure

$$g(\vec{k}') = \int d^3r\, e^{-i\vec{k}'\cdot\vec{r}}\, \psi(\vec{r},0).$$

The wave function at $t=0$ determines $g(\vec{k})$ which in turn determines $\psi(\vec{r},t)$ at all times. As commented earlier, this just reflects the fact that the Schrödinger equation is first order in $\frac{\partial}{\partial t}$.

Even for $V \neq 0$, the Fourier expansion theorem applies, so any square-integrable function can be written as a superposition of plane waves now, however, with time dependent coefficients to be determined,

$$\psi(\vec{r},t) = \int \frac{d^3k}{(2\pi)^3}\, g(\vec{k},t)\, e^{i\vec{k}\cdot\vec{r}} ,$$

$g(\vec{k},t)$ is found from Schrödinger's equation.

For the free particle

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r},t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r},t)$$

$$\Rightarrow \quad i\hbar \frac{\partial}{\partial t} g(\vec{k},t) = \frac{\hbar^2 k^2}{2m} g(\vec{k},t) \quad \text{and}$$

hence

$$g(\vec{k},t) = g(\vec{k})\, e^{-i\omega t} \quad \text{with } \omega = \frac{\hbar k^2}{2m} .$$

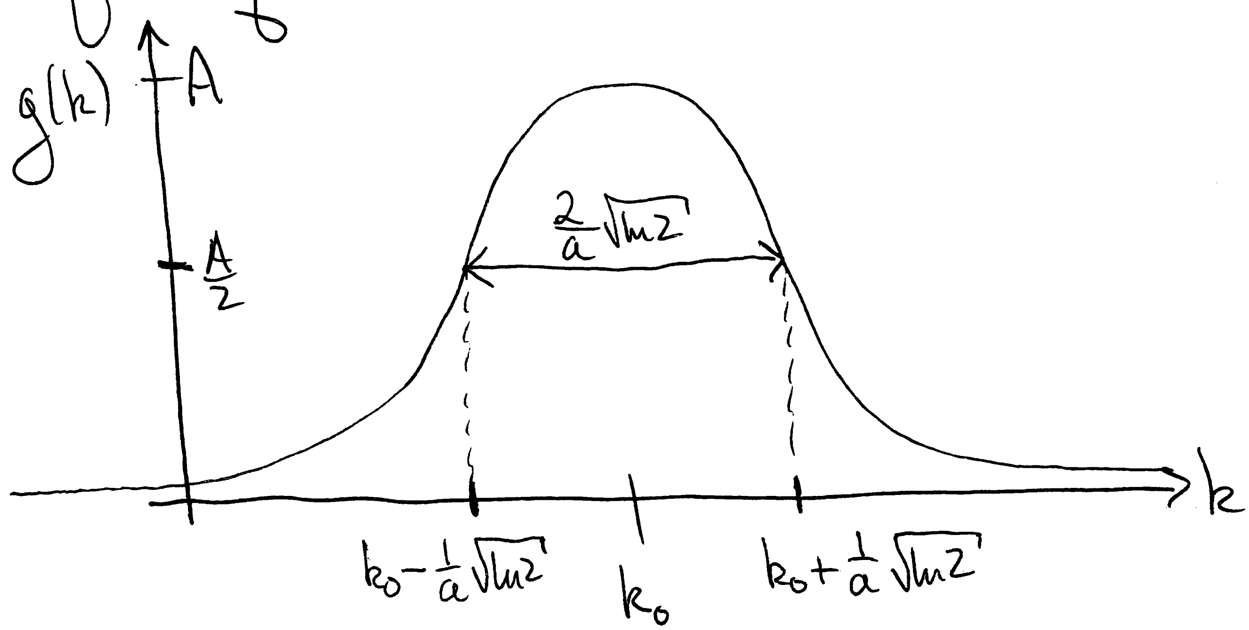
The wave packet solution to the free Schrödinger equation is not in general an eigenfunction of the momentum operator $\vec{p} = -i\hbar\vec{\nabla}$. Such a particle state has a spread in momentum values. As an example let's consider the wave packet in one-dimension that has a Gaussian distribution of momentum values about k_0. Thus

$$\psi(x,t) = \int_{-\infty}^{+\infty} \frac{dk}{2\pi}\, g(k)\, e^{i(kx-\omega_k t)}$$

with

$$g(k) = A e^{-a^2(k-k_0)^2}$$

where A, a, k_0 are constants defining the form of the distribution.



The wave packet is peaked in momentum ($\hbar k$) space about $k = k_0$. As a increases the distribution sharpens about k_0, the particle is said to be localized in momentum space about $\hbar k_0$. The coordinate space wavefunction can be found by completing the square in the exponent to do the integral,

$$\psi(x,t) = A\int_{-\infty}^{+\infty} \frac{dk}{2\pi}\, e^{-a^2(k-k_0)^2 + ikx - \frac{i\hbar k^2}{2m}t} .$$

The exponent is given by

$$-a^2(k-k_0)^2 + ikx - \frac{i\hbar k^2}{2m}t$$

$$= -\left[a^2 + \frac{i\hbar t}{2m}\right]k^2 + (ix + 2a^2k_0)k - a^2k_0^2 .$$

Using the simple identity to complete the square

$$\alpha k^2 + 2\beta k + \gamma = \alpha\left(k + \frac{\beta}{\alpha}\right)^2 - \frac{\beta^2}{\alpha} + \gamma$$

we find

$$-a^2(k-k_0)^2 + i\left(kx - \frac{\hbar k^2}{2m}t\right)$$

$$= -\left(a^2 + \frac{i\hbar t}{2m}\right)\left(k - \frac{\left(\frac{ix}{2} + a^2 k_0\right)}{\left(a^2 + \frac{i\hbar t}{2m}\right)}\right)^2 + \frac{\left(\frac{ix}{2} + a^2 k_0\right)^2}{\left(a^2 + \frac{i\hbar t}{2m}\right)} - a^2 k_0^2$$

$$= -\left(a^2 + \frac{i\hbar t}{2m}\right)\left[k - \hat{k}\right]^2$$

$$- \frac{1}{4\left(a^2 + \frac{i\hbar t}{2m}\right)}\left[x^2 - 2x\frac{k_0 \hbar t}{m} + \frac{2i\hbar t a^2 k_0^2}{m}\right]$$

$$+ \frac{ixk_0 \cancel{\left(a^2 + \frac{i\hbar t}{2m}\right)}}{\cancel{\left(a^2 + \frac{i\hbar t}{2m}\right)}}$$

with $\hat{k} = \dfrac{\frac{ix}{2} + a^2 k_0}{\left(a^2 + \frac{i\hbar t}{2m}\right)}$

$$= -\left(a^2 + \frac{i\hbar t}{2m}\right)(k - \hat{k})^2 + ik_0 x$$

$$- \frac{1}{4\left(a^2 + \frac{i\hbar t}{2m}\right)}\left(x - \frac{\hbar k}{m}t\right)^2 - \frac{i\hbar k_0^2 t\left(a^2 + \frac{i\hbar t}{2m}\right)}{2m\left(a^2 + \frac{i\hbar t}{2m}\right)}$$

Thus we find

$$\boxed{\begin{aligned} &-a^2(k-k_0)^2 + i\left(kx - \frac{\hbar k^2}{2m}t\right) \\ &= -\left(a^2 + \frac{i\hbar t}{2m}\right)(k-\hat{k})^2 + ik_0x \\ &\qquad - \frac{i\hbar k_0^2}{2m}t - \frac{1}{4\left(a^2+\frac{i\hbar t}{2m}\right)}\left(x - \frac{\hbar k_0}{m}t\right)^2 \end{aligned}}$$

The wavefunction becomes

$$\psi(x,t) = A\, e^{\left[ik_0x - \frac{i\hbar k_0^2}{2m}t - \frac{\left(x-\frac{\hbar k_0}{m}t\right)^2}{4\left(a^2+\frac{i\hbar t}{2m}\right)}\right]} \times$$

$$\times \int_{-\infty}^{+\infty} \frac{dk}{2\pi}\, e^{-\left(a^2+\frac{i\hbar t}{2m}\right)(k-\hat{k})^2}.$$

But the Gaussian momentum integral is simply

$$\int_{-\infty}^{+\infty} dk\, e^{-\alpha(k-\hat{k})^2} = \int_{-\infty}^{+\infty} dl\, e^{-\alpha l^2} \qquad (l = k-\hat{k})$$

$$= \sqrt{\frac{\pi}{\alpha}} \qquad (\mathrm{Re}\,\alpha > 0).$$

Hence we find

$$\boxed{\psi(x,t) = \frac{A}{2\sqrt{\pi}} \frac{1}{\sqrt{a^2 + \frac{i\hbar t}{2m}}} \times e^{i\left[k_0 x - \frac{\hbar k_0^2}{2m} t\right]} \, e^{-\frac{\left(x - \frac{\hbar k_0}{m} t\right)^2}{4\left(a^2 + \frac{i\hbar t}{2m}\right)}}}$$

The particle's position probability is given by

$$|\psi(x,t)|^2 = \frac{|A|^2}{4\pi} \frac{1}{\left(a^4 + \frac{\hbar^2 t^2}{4m^2}\right)^{1/2}} e^{-\frac{\left(x - \frac{\hbar k_0}{m} t\right)^2}{2a^2\left(1 + \frac{\hbar^2 t^2}{4m^2 a^4}\right)}}.$$

Defining the function

$$a^2(t) \equiv a^2\left(1 + \frac{\hbar^2 t^2}{4m^2 a^4}\right) \quad \text{with } a(0) = a$$

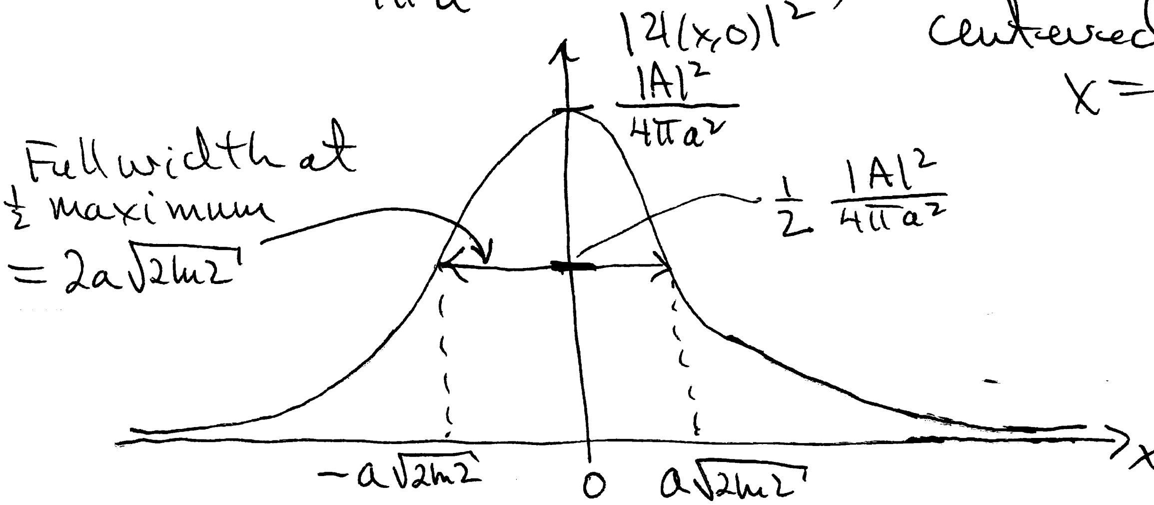
The probability distribution becomes

$$\boxed{|\psi(x,t)|^2 = \frac{|A|^2}{4\pi a\, a(t)}\, e^{-\frac{\left(x-\frac{\hbar k_0}{m}t\right)^2}{2a^2(t)}}}$$

For $t=0$ this yields

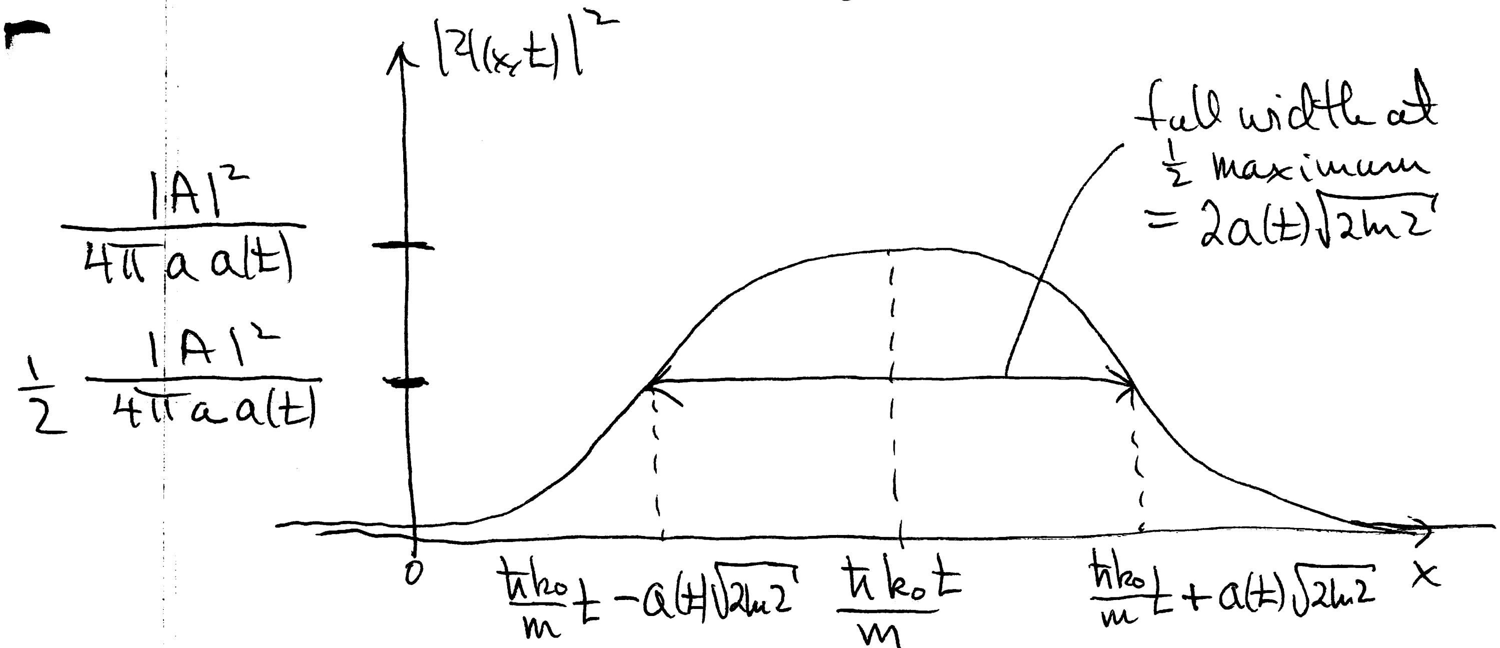
$$|\psi(x,0)|^2 = \frac{|A|^2}{4\pi a^2}\, e^{-\frac{x^2}{2a^2}},$$

a Gaussian centered about $x=0$



Note: the smaller a the more localized in x-space.

Now for $t>0$ the position probability density is still a Gaussian, now peaked about $x = \frac{\hbar k_0}{m}t$,



<u>Remarks:</u>

1) Gaussian distribution of momenta, $g(k)$, leads to a Gaussian spatial distribution for $|\psi|^2$.

2) As postulate 2 implies, $|\psi|^2$ is the position probability density so that the average position, that is mean position is

$$\langle x\rangle = \frac{\int_{-\infty}^{+\infty} dx\; x\,|\psi(x,t)|^2}{\int_{-\infty}^{+\infty} dx\,|\psi(x,t)|^2}$$

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} dx\, x e^{-\frac{(x - \frac{\hbar k_0}{m} t)^2}{2a^2(t)}}}{\int_{-\infty}^{+\infty} dx\, e^{-\frac{(x - \frac{\hbar k_0}{m} t)^2}{2a^2(t)}}}$$

let $y \equiv x - \frac{\hbar k_0}{m} t$ so that

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} dy \left(y + \frac{\hbar k_0}{m} t\right) e^{-y^2/2a^2(t)}}{\int_{-\infty}^{+\infty} dy\, e^{-y^2/2a^2(t)}}.$$

But $\int_{-\infty}^{+\infty} dy\, y\, e^{\frac{-y^2}{2a^2(t)}} = 0$ since the integrand is odd in y.

This yields

$$\boxed{\langle x \rangle = \frac{\hbar k_0}{m} t}$$

The mean value of the particle's position is just the peak's position and it moves like a classical particle with velocity $v = \frac{\hbar k_0}{m} = \frac{P_0}{m}$.

3) The root mean square deviation in the particle's position is defined by

3)
$$\Delta x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle}$$

That is
$$(\Delta x)^2 = \langle (x - \langle x \rangle)^2 \rangle$$
$$= \langle x^2 \rangle - 2\langle x \rangle \langle x \rangle + \langle x \rangle^2$$
$$= \langle x^2 \rangle - \langle x \rangle^2 \, .$$

As for the mean location we have
$$\langle x^2 \rangle = \frac{\int_{-\infty}^{+\infty} dx \, x^2 \, |\psi(x,t)|^2}{\int_{-\infty}^{+\infty} dx \, |\psi(x,t)|^2}$$
$$= \frac{\int_{-\infty}^{+\infty} dy \left[y^2 + \left(\frac{\hbar k_0 t}{m} \right)^2 \right] e^{-\frac{y^2}{2a^2(t)}}}{\int_{-\infty}^{+\infty} dy \; e^{-y^2/2a^2(t)}}$$

But
$$\int_{-\infty}^{+\infty} dy \, y^2 e^{-\beta y^2} = -\frac{\partial}{\partial \beta} \int_{-\infty}^{+\infty} dy \, e^{-\beta y^2}$$
$$= -\frac{\partial}{\partial \beta} \sqrt{\frac{\pi}{\beta}}$$
$$= \frac{\sqrt{\pi}}{2\beta^{3/2}} \, ,$$

which implies

$$\int_{-\infty}^{+\infty} dy\, y^2 e^{-\frac{y^2}{2a^2(t)}} = \sqrt{2\pi}\, a^3(t).$$

So

$$\langle x^2 \rangle = a^2(t) + \left(\frac{\hbar k_0 t}{m}\right)^2$$

Thus

$$(\Delta x)^2 = a^2(t)$$
$$= a^2\left(1 + \frac{\hbar^2 t^2}{4m^2 a^4}\right),$$

As time increases the deviation in position increases, the wave packet is said to spread. This is of course seen also from the graph of $|\Psi|^2$, the full width at half maximum was $2a(t)\sqrt{2\ln 2}$, increasing as time increased.

4) As the wave packet spreads, the height of the peak decreases so that the area under $|\Psi|^2$ is constant. That is the wave packet is indeed square-integrable

$$\int_{-\infty}^{+\infty} dx\, |\Psi(x,t)|^2 = \frac{|A|^2}{4\pi a\, a(t)} \int_{-\infty}^{+\infty} dx\, e^{-\frac{(x - \frac{\hbar k_0}{m} t)^2}{2a^2(t)}}$$

The spreading of the wave packet is expected due to the de Broglie hypothesis dispersion relation $\omega = \frac{\hbar k^2}{2m}$ for each plane wave. That is we know that an electromagnetic wave propagation in vacuum moves with a constant phase velocity c for all frequencies. In a dispersive medium that phase velocity becomes $v = \frac{c}{n(k)}$ with $n(k)$ the index of refraction for the medium. For a free particle $v \equiv \frac{\omega}{k} = \frac{\hbar k}{2m}$ depends on k and so acts like wave propagation in a dispersive medium, hence the spreading of the wave packet.

4)
$$= \frac{|A|^2}{4\pi a\, a(t)} \sqrt{\pi}\, 2^{1/2} a(t)$$

$$= \frac{|A|^2}{\sqrt{8\pi}\, a}.$$

Thus we see that the superposition of plane waves with a Gaussian weight leads to a normalizable wavefunction as required.

So it is seen from this example that we can construct physical (normalizable) wavefunctions that are localized to some degree in both momentum and position. If a particle state with approximately a given momentum is desired we ~~can~~ peak the distribution in momentum space more sharply (i.e. let a increase) for a particle state more localized in position we spread the momentum distribution, that is include more plane waves with different k in our sum (i.e. let a decrease). At all times the state is normalizable.

Of course it is mathematically quite tedious to manipulate these physical wave packet states in any calculation, so we will resort to using plane wave states of a single frequency instead. If confusion arises in a calculation, we can always return to using wave packets, and then, at the end of the calculation take the plane wave limit. In particular recall the Gaussian representation for the Dirac δ-function

$$2\pi\,\delta(k-k_0) = \lim_{a\to\infty} \sqrt{4\pi}\, a\, e^{-a^2(k-k_0)^2} .$$

Thus if we choose the normalization factor A to be $A = \sqrt{4\pi}\, a$ then

$$\lim_{a\to\infty} g(k) = 2\pi\,\delta(k-k_0) \quad \text{and}$$

$$\psi(x,t) = \int_{-\infty}^{+\infty} \frac{dk}{(2\pi)}\, g(k)\, e^{i(kx-\omega t)}$$

$$\xrightarrow[a\to\infty]{} e^{i(k_0x-\omega_{k_0}t)}$$

the single plane wave with momentum $\hbar k_0$ and energy $\hbar\omega_{k_0} = \frac{\hbar^2 k_0^2}{2m}$.

Of course the wave-function is no longer normalizable $\int_{-\infty}^{+\infty} dx\, |\psi(x,t)|^2 = \frac{|A|^2}{\sqrt{8\pi}\, a} = a\sqrt{2\pi} \xrightarrow[a\to\infty]{} \infty$

as expected. However the relevant observables will be finite in this limit since this normalization factor is cancelled from numerator and denominator, as in the calculation of energy, say, before the limit $a\to\infty$ is taken!

1.3.3. Expectation Values

Since $|\psi(\vec{r},t)|^2$ is the position probability density (let $\int d^3r\, |\psi(\vec{r},t)|^2 = 1$ for simplicity) the expectation value of any function, $f(\vec{r})$, of position is given by

$$\langle f \rangle \equiv \int d^3r\, f(\vec{r})\, |\psi(\vec{r},t)|^2 .$$

Further, any square-integrable wave function (even for $V \neq 0$) can be Fourier expanded

$$\psi(\vec{r},t) = \int \frac{d^3k}{(2\pi)^3}\, e^{i\vec{k}\cdot\vec{r}}\, g(\vec{k},t) .$$