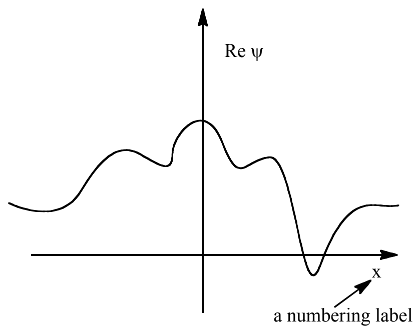
Momentum Representation

The majority of our work is in the coordinate representation which specifies the evolving state of the system through a wavefunction expressed in space and time

$$\Psi(x,t) = \langle x \mid \Psi \rangle$$

Here, $|x\rangle$ is a label which refers to the complete orthonormal basis set, $\langle x|x'\rangle = \delta(x-x')$ and $\sum_x |x\rangle\langle x| = 1$, which forms a continuum of vectors that map to all points in space. We can do this because the operator $\hat{x}$ is Hermetian, so that its eigenstates form a complete orthonormal basis. We can therefore completely specify the wavefunction in terms of the amplitude of each *x* component.



For a one-dimensional problem in the coordinate representation, we replace the classical variable *x* with the operator $\hat{x}$ and the classical variable *p* with the operator $-i\hbar\frac{\partial}{\partial x}$. An observable is calculated as an expectation value of an operator expressed in these variables:

$$\langle A(x,p)\rangle \rightarrow \int_{\infty}^{+\infty} dx\, \psi^*(x) A\left(x, -i\hbar\frac{\partial}{\partial x}\right)\psi(x)$$

$$\langle x\rangle = \int_{-\infty}^{+\infty} dx\, \psi^*(x)\, x\, \psi(x)$$

$$\langle p\rangle = \int_{-\infty}^{+\infty} dx\, \psi^*(x)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x)$$

Unlike classical mechanics, we cannot uniquely specify both $\hat{p}$ and $\hat{x}$ for a particle. We have already noted that eigenstates of $\hat{x}$ are not eigenstates of $\hat{p}$. It is therefore possible to define a new basis set $|p\rangle$ which describes the wavefunction in the momentum representation: $\Psi(p,t) = \langle p \mid \Psi\rangle$. $|p\rangle$ is also a complete orthonormal basis, $\langle p|p'\rangle = \delta(p-p')$, $\Sigma|p\rangle\langle p| = 1$ which allows us to describe the momentum distribution for a particle. In the momentum representation we will replace:

$$p \rightarrow \hat{p} = \frac{\hat{k}}{\hbar}$$
$$x \rightarrow i\hbar\frac{\partial}{\partial p}.$$

Naturally, we will want to be able to transform from one basis to another, and this transformation is expressed through

$$\langle x | p \rangle = \langle p | x \rangle^* = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{p}{\hbar}x}$$

since x and p form a continuum, we can replace the sum over basis vectors in the completeness expression with an integral

$$1 = \sum_x |x\rangle\langle x| \to \int_{-\infty}^{\infty} dx |x\rangle\langle x|$$

$$1 = \sum_p |p\rangle\langle p| \to \int_{\infty}^{-\infty} dp |p\rangle\langle p|.$$

This allows us to transform the wavefunction in the position representation to momentum representation with a Fourier transform, or vice versa:

$$\psi(p) = \langle p | \psi \rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dx \langle p | x \rangle \langle x | \psi \rangle$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dx \, \psi(x) e^{-ipx/\hbar}$$

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dp \, \psi(p) \, e^{ipx/\hbar}$$

We will use the wavevector notation where $k = \dfrac{p}{\hbar}$ in three dimensions:

$$\psi(x) = \frac{1}{(2\pi)^{3/2}} \int_{-\infty}^{+\infty} \Phi(k) e^{ikx} d^3k$$

$$\Phi(k) = \frac{1}{(2\pi)^{3/2}} \int_{-\infty}^{+\infty} \psi(x) e^{-ikx} d^3x \qquad (39)$$

Returning to our earlier discussion of the free particle the eigenfunctions of $\hat{p} = -i\hbar(\partial/\partial x)$ are

$$\psi_k(x) = \frac{1}{\sqrt{2\pi}} e^{-ikx}$$

where $\hbar k = p$. This is the coordinate representation, whereas the momentum representation is

$$\psi(k) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dx' e^{ikx'} \psi_k(x) = \frac{1}{\sqrt{2\pi\hbar}} ik\delta(x' - x).$$

We can now show:

$$\int_{-\infty}^{+\infty} dp \, \Phi^*(p) \Phi(p) = \int_{-\infty}^{+\infty} dx \, \Psi^*(x) \Psi(x)$$

$$\langle p \rangle = \int_{-\infty}^{+\infty} dp \, \Phi^*(p) \, p \, \Phi(p)$$

$$\langle x \rangle = \int_{-\infty}^{+\infty} dp \, \Phi^*(p) \left(-i\hbar \frac{\partial}{\partial p} \right) \Phi(p)$$

$$i\hbar \frac{\partial \Phi}{\partial t} = \hat{H}_p \Phi$$

$$\hat{H}_p = \frac{p^2}{2m} + V\left(i\hbar \frac{\partial}{\partial p} \right)$$

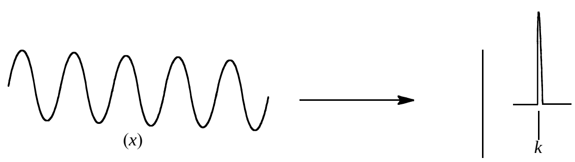
As an example, consider the Harmonic Oscillator. The wavefunction in momentum and coordinate space are the same, but the roles of the kinetic and potential energy are interchanged.

$$\hat{H} = -\frac{1}{2}\frac{\hbar^2}{m}\frac{\partial^2}{\partial x^2} + \frac{1}{2} m\omega_0^2 x^2$$

$$\hat{H}_p = -\frac{1}{2}\hbar^2 m\omega_0^2 \frac{\partial^2}{\partial p^2} + \frac{1}{2}\frac{p^2}{m}$$

Note these form of these equations, and their solutions, are the same when equating the force constant with the inverse mass $m\omega_0^2$ $\rightarrow m^{-1}$ and $x \rightarrow p$. To solve this, the boundary conditions are also similar. Since Ψ vanishes for large *x* in the coordinate representation, Φ must vanish for large *p* in the momentum representation. One can show that

$$\Phi_n(p) = \frac{i^n}{\sqrt{m\omega_0}} \psi\left(\frac{p}{m\omega_0} \right)$$



Free Particle Wavepacket

The momentum representation is particularly useful for describing the propagation of free particles in time and space. In order to localize the particle in time and space we can construct a minimum uncertainty wavepacket, using a Gaussian distribution in *k* space. At the initial time point *t*=0, we set

$$\Phi(k) = e^{-\alpha(k-k_0)^2} \quad \Phi(k) = e^{-(k-k_0)^2/2\Delta k^2} \tag{40}$$

Here k_0 is the most probable wavevector, whereas the spread of wavevectors are described by Δk. Such a distribution is pictured in Figure xx. The wavepacket in coordinate space is obtained from

$$\psi(x,t) = \int_{-\infty}^{+\infty} dk\, \Phi(k)\, e^{ikx - i\omega_k t} \tag{41}$$

where

$$\omega_k = kc = \frac{\hbar k^2}{2m}. \tag{42}$$

So, from eq. (41), we see that in space, the wavepacket is also initially a Gaussian localized in space with a width $1/\Delta k$:

$$\psi\left(x,0\right) = \sqrt{2\pi}\,\sigma\, e^{ik_0 x}\, e^{-\Delta k^2 x^2/2} \tag{43}$$

If we expand (42) about k_0

$$\begin{aligned}\omega_k &= \omega_0 + \left.\frac{\partial\omega}{\partial k}\right|_{k_0}\left(k-k_0\right)+\cdots \\ &= \omega_0 + v_g\left(k-k_0\right)\end{aligned} \tag{44}$$

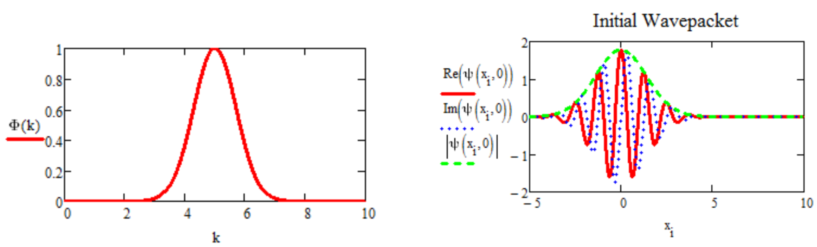
then we can use (41) to obtain

$$\psi\left(x,t\right)=\sqrt{2\pi}\,\sigma\, e^{i(k_0x-\omega_0 t)}\; e^{-\Delta k^2\left(x-v_g t\right)^2/2} \tag{45}$$

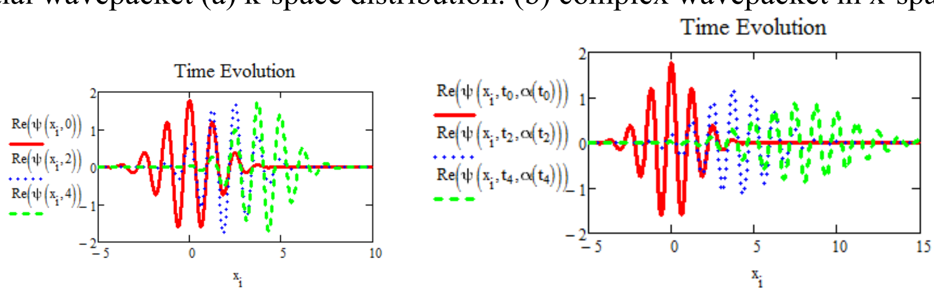
and the observed probability distribution

$$\left|\psi\right|^2 = 2\pi\sigma^2 e^{-\Delta k^2\left(x-v_g t\right)^2/2} \tag{46}$$

The wavepacket propagates as a Gaussian with group velocity v_g and width α. This wavepacket if plotted in Fig. xx corresponding to the wavevector distribution in Fig. xx. Whereas the k space wavepacket was a simple Gaussian, in coordinate representation, the wave character of the particle is apparent from the complex phase factor. For the case that there is dispersion, as is usually the case in dissipative media, $\beta = (\partial^2\omega/\partial k^2)_{k_0} \neq 0$, then one can add the third term to expansion of ω_k in eq. (44). Now one can substitute $\Delta k^2 \to \Delta k^2/\left(1+2i\Delta k^2\beta t\right)$ in eqn. (45).



Initial wavepacket (a) k-space distribution. (b) complex wavepacket in x-space.



Time-evolution of wavepacket above: (c) no dispersion, (d) with dispersion.