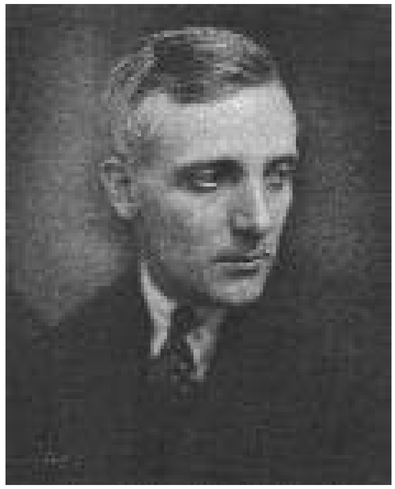


Leon Brillouin (1889–1969)
Author of *Wave Propagation in Periodic Structures* (1946)

3

Position and momentum space

3.1 Group and phase velocity

Consider a sinusoidal plane wave is propagating along the x axis without any distortion. The wave can be represented by the wave function

$$\Psi(x, t) \quad = \quad \Psi(x - v_{\text{ph}}\, t) \tag{3.1}$$

where v_{ph} is the phase velocity of the wave. This wave possesses translational symmetry, since the wave at the time t is identical to the wave at $t = 0$ shifted on the x axis by an amount of $v_{\text{ph}}t$. For example, a sinusoidal plane wave with amplitude A is given by

$$\Psi(x, t) \quad = \quad A \cos(k\, x - \omega\, t). \tag{3.2}$$

The locations of constant phase are given by

$$k\, x \; - \; \omega\, t \quad = \quad \text{const.} \tag{3.3}$$

Differentiation of the position with respect to t yields the ***phase velocity***

$$\boxed{v_{\text{ph}} \quad = \quad \frac{\mathrm{d}x}{\mathrm{d}t} \quad = \quad \frac{\omega}{k}} \tag{3.4}$$

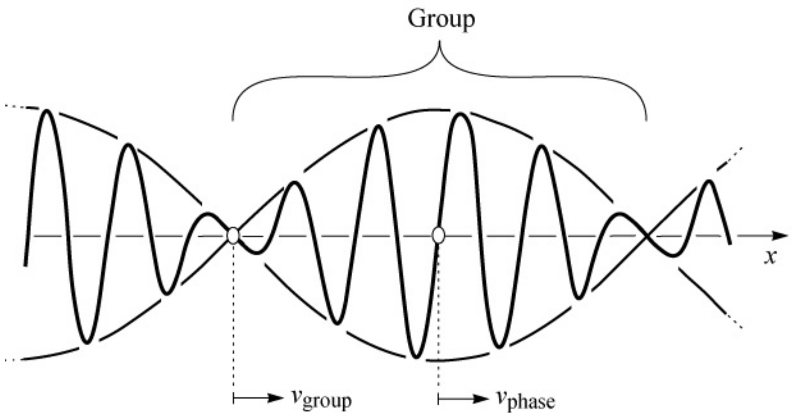


Fig. 3.1. Example for a group of waves propagating along the x-direction. An entire group of wavelets propagates with group velocity v_{group}. Individual wavelets propagate with phase velocity v_{phase}.

Groups of waves, also called wave packets, can propagate with velocities *different* from the phase velocity. A group of waves is illustrated in ***Fig***. 3.1 by a superposition of two sinusoidal waves with similar angular frequency:

$$\Psi(x,t) \;=\; A\cos(k_1\, x - \omega_1\, t) \;+\; A\cos(k_2\, x - \omega_2\, t). \tag{3.5}$$

We define

$$\omega_1 \;=\; \omega - \Delta\omega \qquad \text{and} \qquad \omega_2 \;=\; \omega + \Delta\omega \tag{3.6}$$

$$k_1 \;=\; k - \Delta k \qquad \text{and} \qquad k_2 \;=\; k + \Delta k\,. \tag{3.7}$$

Trigonometric modification yields

$$\Psi(x,t) \;=\; 2\,A\cos(\omega\, t - k\, x)\;\cos(\Delta\omega\, t - \Delta k\, x) \tag{3.8}$$

with $\Delta\omega \ll \omega$ one can interpret the wave function as a rapidly oscillating term $\cos(\omega\, t - k\, x)$ and a slowly oscillating term $\cos(\Delta\omega\, t - \Delta k\, x)$ which in turn modulates the amplitude of the rapidly oscillating term. The zeros of the rapidly oscillating term propagate with the phase velocity $v_{ph} = \omega / k$. On the other hand, the phase of the slowly varying term, *i. e.* the wave group, propagates at a velocity $v_{gr} = \Delta\omega / \Delta k$. Thus, for infinitesimal small quantities of $\Delta\omega$ and Δk one obtains the ***group velocity***

$$\boxed{v_{gr} \;=\; \frac{d\omega}{dk}} \tag{3.9}$$

The group velocity is the velocity at which the wave packets or wavelets propagate in space. The phase velocity can be smaller, equal, or larger than the group velocity. If the phase velocity is larger ($v_{ph} > v_{gr}$), then the wavelets build up at the back end of the group, propagate through the group, and disappear at the front of the group. If the phase velocity is smaller ($v_{ph} < v_{gr}$), then the wavelets are building up at the front end of the group and disappear at the rear end of the group.

In media in which the phase velocity is independent of the frequency of the wave, the phase velocity and group velocity are identical

$$v_{ph} = v_{gr} = \frac{\omega}{k} = \frac{d\omega}{dk}. \tag{3.10}$$

Such media are called ***nondispersive media***. Vacuum, and with good approximation also air, are such nondispersive media. The velocity of electromagnetic waves in vacuum and air is $c = 2.99 \times 10^8$ m / s and this velocity is independent of the frequency of the wave.

If, however, the phase velocity depends on ω then $v_{ph} \neq v_{gr}$. Media in which $v_{ph} \neq v_{gr}$ are called ***dispersive media***. The group velocity in dispersive media can be written as

$$v_{gr} = v_{ph} + k \frac{dv_{ph}}{dk}. \tag{3.11}$$

The validity of this equation can be verified by insertion of $v_{ph} = \omega / k$. Using $k = 2\pi / \lambda$ and $d\lambda^{-1} = -\lambda^{-2}\, d\lambda$, one can show that

$$v_{gr} = v_{ph} - \lambda \frac{dv_{ph}}{d\lambda}. \tag{3.12}$$

It has been shown that a well-defined group of waves (a *wave packet*) moves with the group velocity. In the classical limit, the group velocity is identical to the propagation velocity of the classical particle described by the wave-packet, *i. e.*

$$v_{gr} = v_{classical}. \tag{3.13}$$

This requirement is called the ***correspondence principle***. The correspondence principle, which is due to Bohr (1923), postulates a detailed analogy between quantum mechanics and classical mechanics. Specifically it postulates that the results of quantum mechanics merge with those of classical mechanics in the classical limit, *i. e.* for large quantum numbers. Using the definitions of group velocity and of the classical velocity one obtains

$$\frac{d\omega}{dk} = \frac{p}{m}. \tag{3.14}$$

Substitution of k by using the de Broglie relation ($p = \hbar k$) and subsequent integration yields

$$\boxed{E_{kin} = \hbar\omega = \frac{p^2}{2m}} \tag{3.15}$$

which is the famous ***Planck relation***. The Planck relation further illustrates the dualism of particles and waves. A particle with momentum p oscillates at an angular frequency ω given by the Planck relation. On the other hand, a wave with angular frequency ω has a momentum p. The kinetic energy $p^2/ 2m$ of the particle coincides with the quantum energy $\hbar\omega$ of the wave representing that particle.

Exercise. ***Phase and group velocity***. The experiment described here elucidates the properties of waves, in particular the phase and group velocity. Go to a local pond and throw stones into the water. Watch the water waves created. Several properties of waves can be identified.

The water waves are confined to the surface of the water. What are the curves of constant phase?

Identify the phase and group velocity of the waves. Which of the two velocities is higher? Make a guess for the ratio of v_{ph} / v_{gr}.

Assume that the distance from the point where a stone enters the water to the shore is x. Can the time it takes for the wave to reach shore be expressed in terms of phase or group velocity and the distance x?

Solution: The curves of constant phase are concentric circles. The phase velocity is higher than the group velocity. Note that individual wavelets appear at the trailing edge of the wave group, move forward through the group of waves, and disappear at the leading edge of the group. The ratio of phase-to-group velocity is given by $v_{ph} / v_{gr} \approx 2.0$. The time that it takes the wave to reach the shore is given by $t = x / v_{gr}$.

3.2 Position-space and momentum-space representation, and Fourier transform

According to the 2nd Postulate, the stationary wave function $\psi(x)$ has a clear physical meaning: The probability density is given by the product of the wave function and its complex conjugate, *i. e.* $\psi^*(x)\ \psi(x)$. The wave function $\psi(x)$ can be also represented in momentum space. The momentum-space representation is designated as the wave function in momentum space, $\Phi(p)$. The momentum-space wave function is not a new wave function, but just another representation of a wave function with the same physical content. The two representations are related by the Fourier transform. The momentum space representation of the wave function is obtained from the wave function $\psi(x)$ by the Fourier transform

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x)\, e^{-ipx/\hbar}\, dx \tag{3.16}$$

The wave function in real space is calculated from the wave function in momentum space by the inverse Fourier transform

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Phi(p)\, e^{ipx/\hbar}\, dp \tag{3.17}$$

where $\Phi(p)$ is the amplitude of the momentum space wave function at the momentum p. The Fourier transform provides a unique relationship between the momentum space and position space representation of a particle. That is, for a specific wave function $\psi(x)$ there is only one representation in momentum space $\Phi(p)$.

Another property of the Fourier transform is that the normalization condition holds for the position and momentum space representation. If $\psi(x)$ is normalized, then $\Phi(p)$ is normalized as well.

$$\int_{-\infty}^{\infty} \psi^*(x)\, \psi(x)\, dx = \int_{-\infty}^{\infty} \Phi^*(p)\, \Phi(p)\, dp = 1 \tag{3.18}$$

The Fourier transform (Eqs. 3.16 and 3.17) will not be proved here. The interested reader is referred to the literature (see, for example, Kroemer, 1994). The normalization condition (Eq. 3.18) can be proved by using the Fourier transform.

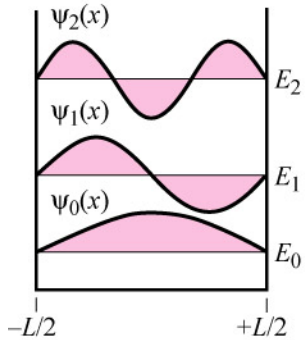
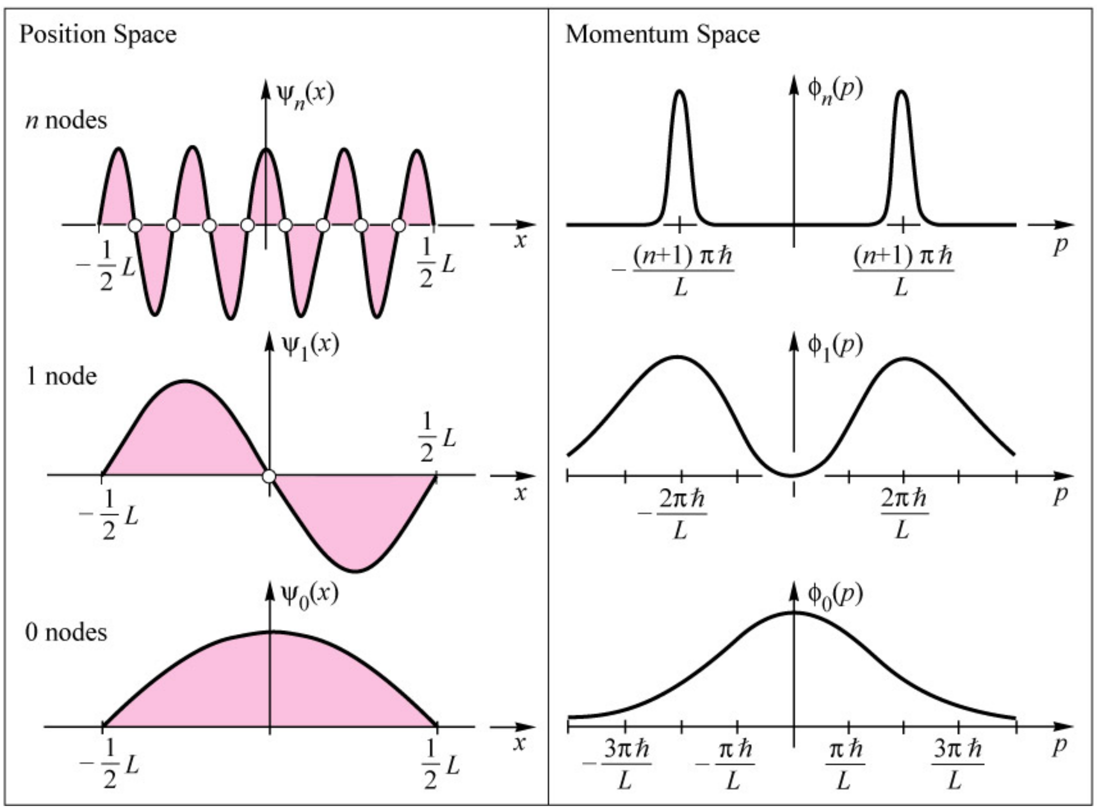


Fig. 3.2. Below: Position space representation and momentum space representation of three wave functions $\psi_0(x)$, $\psi_1(x)$, $\psi_n(x)$. The subscript n refers to the number of nodes (nodes at $x = \pm\ (1/2)\ L$ are not counted). Left: The three lowest wave functions $\psi_0(x)$, $\psi_1(x)$, $\psi_3(x)$ of an infinite quantum well.



3.3 Illustrative example: Position and momentum in the infinite square well

One of the simplest quantum mechanical potentials is a square well with infinitely high walls. It will be seen in the Section on Schrödinger's equation how to find the wave functions in the infinite square well potential. Here we are not concerned about how to solve Schrödinger's equation and how to find the wave function. The solutions are shown in ***Fig***. 3.2. The solutions have discrete energies and the wave functions are of sinusiodal shape. The wave functions of the lowest state (n = 0) and the first excited state (n = 1) are given by:

$$\psi_0(x) \quad = \quad \sqrt{\frac{2}{L}} \quad \cos\left(\frac{\pi}{L}\,x\right) \qquad\qquad \left(\left|\,x\,\right| \ < \ \frac{1}{2}\,L\right) \qquad (3.19)$$

$$\psi_1(x) = \sqrt{\frac{2}{L}} \cos\left(\frac{2\pi}{L} x + \frac{\pi}{2}\right) \qquad \left(|x| < \frac{1}{2} L\right) \tag{3.20}$$

For the *n*th state, the wave function is given by

$$\psi_n(x) = \sqrt{\frac{2}{L}} \cos\left(\frac{(n+1)\pi}{L} x + \frac{n\pi}{2}\right) \quad \left(|x| < \frac{1}{2} L\right) \tag{3.21}$$

Note that these wave functions are normalized. Also note that the wave functions are spatially confined to $|x| < (1/2)L$. The magnitude of the wave functions is zero in the barriers, *i. e.*, it is $\psi_n(x) = 0$ for $|x| \geq (1/2)L$.

The Fourier-transform of Eq. (3.16) is used to obtain the momentum space representations of the wave functions. For the wave function with zero nodes, $\psi_0(x)$, one obtains,

$$\Phi_0(p) = \int_{-\infty}^{\infty} \psi_0(x)\, e^{-\mathrm{i}px/\hbar}\, \mathrm{d}x$$
$$= \sqrt{\frac{L}{\pi\hbar}} \left[\left(\frac{1}{\pi - pL/\hbar}\right) \cos\left(\frac{L}{2\hbar} p\right) + \left(\frac{1}{\pi + pL/\hbar}\right) \cos\left(\frac{L}{2\hbar} p\right)\right]. \tag{3.22}$$

For a wave function with n nodes, $\psi_n(x)$, one obtains

$$\Phi_n(p) = \int_{-\infty}^{\infty} \psi_n(x)\, e^{-\mathrm{i}px/\hbar}\, \mathrm{d}x$$
$$= \frac{1/2}{\sqrt{\pi L \hbar}} \left[\frac{1}{\mathrm{i}\,\alpha}\left(\mathrm{i}^{n+1}\, \mathrm{e}^{-\mathrm{i}\frac{pL}{2\hbar}} - \mathrm{i}^{-(n+1)}\, \mathrm{e}^{\mathrm{i}\frac{pL}{2\hbar}}\right) + \frac{1}{\mathrm{i}\,\beta}\left(\mathrm{i}^{-(n+1)}\, \mathrm{e}^{-\mathrm{i}\frac{pL}{2\hbar}} - \mathrm{i}^{(n+1)}\, \mathrm{e}^{\mathrm{i}\frac{pL}{2\hbar}}\right)\right]. \tag{3.23}$$

where $\alpha = (n+1)(\pi/L) - (p/\hbar)$ and $\beta = -(n+1)(\pi/L) - (p/\hbar)$. The momentum representation $\psi(p)$ is shown for zero, one, and n nodes ($n >> 1$) on the right-hand side of ***Fig***. 3.2. The momentum representation has several interesting aspects. First, $\Phi_n(p)$ is a symmetric distribution with respect to p. Consequently, the expectation value of the momentum is zero, since positive and negative momenta compensate one another. The momentum expectation value can be calculated according to the 5th Postulate using the momentum operator given in the 4th Postulate:

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, \frac{\hbar}{\mathrm{i}} \frac{\mathrm{d}}{\mathrm{d}x}\, \psi(x)\, \mathrm{d}x\,. \tag{3.24}$$

The evaluation of this integral gives indeed $\langle p \rangle = 0$. Second, the momentum representation has two maxima, one at $p = +(n+1)\,\pi\hbar/L$ and another one at $p = -(n+1)\,\pi\hbar/L$. The two-maxima are increasingly pronounced with increasing number of nodes of the wave function. We interpret the *standing wave* $\psi_n(x)$ as a *superposition of two waves*, one propagating in *negative* and another one in *positive* x direction. Returning from the wave-oriented viewpoint to the particle-oriented viewpoint, the wave function $\psi_n(x)$ represents a particle that is propagating back and forth (oscillating) between the boundaries $\pm (1/2)\,L$ on the x axis. The absolute value of the momentum of the oscillating particle is centered at $p = (n+1)\,\pi\,\hbar\,/\,L$, as stated above. That is, the particle represented by the wave function oscillates between the boundaries $+ (1/2)\,L$ *and* $-(1/2)\,L$. Note, however, that the expectation value of the momentum of the oscillating particle is $\langle p \rangle = 0$.

To further visualize the properties of the particle, we note that the particle is represented by a sinusoidal wave function which is confined to $-(1/2)\,L < x < +(1/2)\,L$, and has n nodes as shown in the lower left part of ***Fig***. 3.2. The wavelength of the particle is given by $\lambda = 2\,L\,/\,(n+1)$. (Strictly speaking, a wavelength can only be attributed to a wave which is strictly periodic, and which is not confined to a certain region) The instantaneous momentum of the particle is given by the de Broglie relationship $p = \hbar\,k = 2\,\pi\,\hbar\,/\,\lambda$. Inserting the wavelength into this equation yields the momentum of the particle as

$$p \;=\; \frac{(n+1)\,\pi\,\hbar}{L}\;. \tag{3.25}$$

This momentum is in fact the maximum of the momentum distribution obtained from the Fourier transform as shown in ***Fig***. 3.2.

The momentum space representation has, as already mentioned, the same physical content as the position space representation. The expectation values of dynamical variables can be calculated not only from the position space representation (5th Postulate), but also in the momentum space representation. That is, the expectation value of the dynamical variable ξ can be also obtained from the momentum space representation

$$\langle \xi \rangle \;=\; \int_{-\infty}^{\infty} \Phi^*(p)\,\xi_{\mathrm{op}}\,\Phi(p)\,\mathrm{d}p \tag{3.26}$$

where ξ_{op} is the operator corresponding to the dynamical variable ξ. We proceed to prove this equation for one specific variable, namely the momentum p. We start with the 3rd and 5th Postulate to determine the momentum expectation value

$$\langle p \rangle \;=\; \int_{-\infty}^{\infty} \psi^*(x)\;\frac{\hbar}{\mathrm{i}}\;\frac{\mathrm{d}}{\mathrm{d}x}\;\psi(x)\,\mathrm{d}x\,. \tag{3.27}$$

The wave functions can be represented in momentum space using the Fourier transform of Eq. (3.17):

$$\langle p \rangle \;=\; \frac{1}{2\,\pi\,\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \Phi^*(p')\,\mathrm{e}^{-\mathrm{i}p'x/\hbar}\left(\frac{\hbar}{\mathrm{i}}\,\frac{\mathrm{d}}{\mathrm{d}x}\right)\Phi(p)\,\mathrm{e}^{\mathrm{i}px/\hbar}\,\mathrm{d}x\,\mathrm{d}p\,\mathrm{d}p'\,. \tag{3.28}$$

The equation can be simplified by differentiating $\mathrm{e}^{\mathrm{i}px/\hbar}$ with respect to x, that is

$$\frac{\mathrm{d}}{\mathrm{d}x}\, \mathrm{e}^{\mathrm{i}px/\hbar} \;=\; \frac{\mathrm{i}\, p}{\hbar}\, \mathrm{e}^{\mathrm{i}px/\hbar} \,. \tag{3.29}$$

Introducing this result into Eq. (3.28) yields

$$\langle p \rangle \;=\; \frac{1}{2\,\pi\,\hbar} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Phi^*(p')\, \mathrm{e}^{-\mathrm{i}p'x/\hbar}\; p\, \Phi(p)\, \mathrm{e}^{\mathrm{i}px/\hbar}\; \mathrm{d}x\, \mathrm{d}p\, \mathrm{d}p' \tag{3.30}$$

The functional dependence of the integrand on x is now known explicitly and therefore the integration over x is done first. Employment of the following relation for the Dirac-delta function,

$$\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}(p-p')x/\hbar}\, \mathrm{d}x \;=\; 2\,\pi\,\delta\!\left(\frac{p-p'}{\hbar}\right) \;=\; 2\,\pi\,\hbar\,\delta(p-p') \tag{3.31}$$

yields

$$\langle p \rangle \;=\; \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Phi^*(p')\; p\, \Phi(p)\, \delta(p-p')\, \mathrm{d}p\, \mathrm{d}p' \,. \tag{3.32}$$

Integration over p' finally yields the momentum expectation value

$$\langle p \rangle \;=\; \int_{-\infty}^{\infty} \Phi^*(p)\; p\, \Phi(p)\, \mathrm{d}p \tag{3.33}$$

This equation is, for $\xi_{\mathrm{op}} = p$, identical with Eq. (3.26), which concludes the proof. The dynamical variable *momentum* corresponds to the operator $(\hbar / \mathrm{i})\,(\mathrm{d} / \mathrm{d}x)$ in position space and to the operator p in momentum space. What has just been shown for the momentum operator applies to all quantum mechanical operators: The expectation value of a dynamical variable can be calculated in the position or momentum space representation of the wave function by using the position or momentum space representation of the operator corresponding to the dynamical variable.