Wave Packets

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In quantum mechanics one describes a particle by a wave packet. Conceptually a wave packet may be first studied in one dimension. The generalization to three dimensions is straightforward and will be dealt with in a separate section.

1 One dimensional wave packet

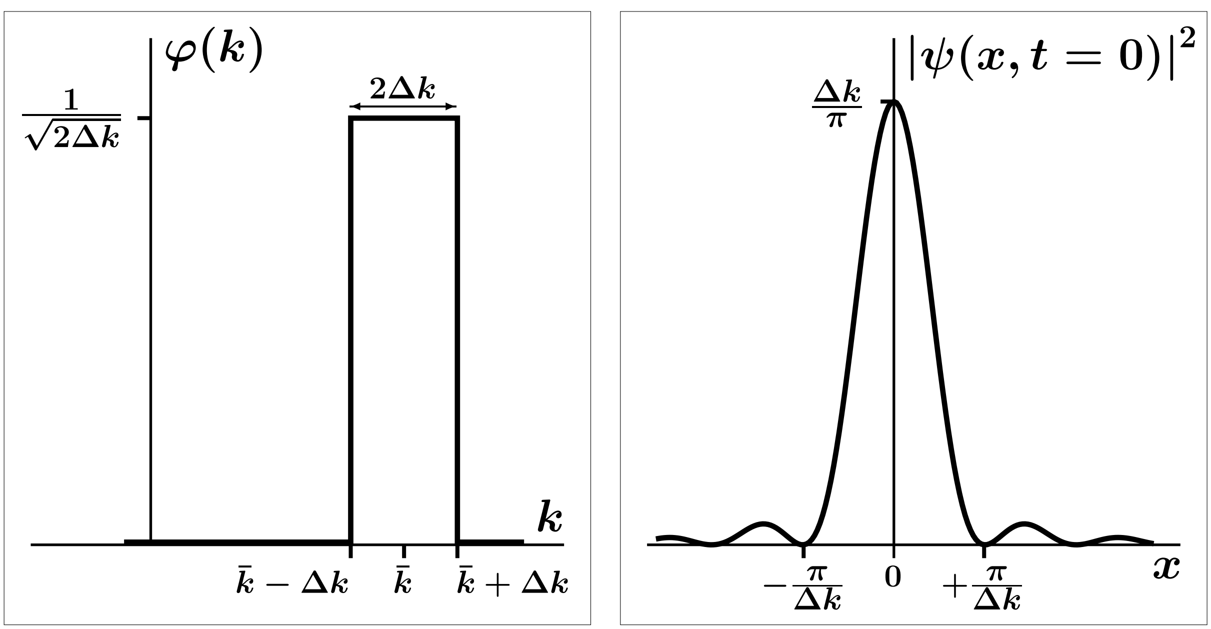
Let us begin by studying an example: We indicate the position parameter in one dimension by x and the time by t. Let us assume that at the instant $t = 0$ a wave packet is given by the following expression (*Fourier expansion*):

$$\psi(x, t = 0) \;=\; \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\; \varphi(k) e^{ikx} \quad . \tag{1}$$

So, once the Fourier transform φ is specified we have an explicit example. The interpretation of the wave packet ψ, shown in formula (1), is the usual, *i.e.* the probability $\mathcal{P}$ to find the particle, described by ψ, at the instant $t = 0$ at the position x is given by the square of the modulus of $\psi(x, t = 0)$ according to:

$$\mathcal{P}(x, t = 0) \;=\; |\psi(x, t = 0)|^2 \quad . \tag{2}$$

The example we will study here for φ, defined in formula (1), is a function of k which peaks around a certain value $k = \bar{k}$ and which vanishes rapidly for large values of $|k|$. For the sake of calculational simplicity we choose a Fourier transform which vanishes everywhere at the k-axis except for a small interval where it has a constant value different from zero, as is shown in figure (1a). In formula, the example for $\varphi(k)$ depicted in figure (1a), is



(a) (b)

Figure 1: (a) The Fourier transform in one dimension of a wave packet which differs from zero only in a small region of width $2\Delta k$ around a central value $k = \bar{k}$. (b) The corresponding wave packet at the instant $t = 0$.

represented by

$$\varphi(k) \;=\; \frac{1}{\sqrt{2\Delta k}}\;\theta\left(\left(k-\bar{k}\right)^2-(\Delta k)^2\right) \;=\; \begin{cases} \dfrac{1}{\sqrt{2\Delta k}} & ,\left|k-\bar{k}\right| \leq \Delta k \\ 0 & ,\left|k-\bar{k}\right| > \Delta k \end{cases} \tag{3}$$

The wave packet ψ which according to equation (1) follows for the above choice of Fourier transform φ can readily be determined to be given by

$$\psi(x,t=0) \;=\; \frac{1}{\sqrt{\pi\Delta k}}\; e^{i\bar{k}x}\;\frac{\sin\left(\Delta k\; x\right)}{x} \quad , \tag{4}$$

the probability distribution of which expression is depicted in figure (1b).

For completeness, let us go through the calculations which lead from formula (3), for our choice of Fourier transform, to expression (4): First notice that φ, given in formula (3), is normalized according to

$$\int_{-\infty}^{\infty} dk\;\left|\varphi(k)\right|^2 \;=\; \int_{\bar{k}-\Delta k}^{\bar{k}+\Delta k} dk\;\frac{1}{2\Delta k} \;=\; 1 \quad . \tag{5}$$

This has as a consequence that the wave packet ψ, given in equation (1), is automatically normalized, which expresses the fact that the probability to find the particle somewhere along the x-axis equals 1 and can be seen from

$$\begin{aligned}
\int_{-\infty}^{\infty} dx\;\left|\psi(x,t=0)\right|^2 \;&=\; \int_{-\infty}^{\infty} dx\;\psi^*(x,t=0)\psi(x,t=0) \;= \\
&= \int_{-\infty}^{\infty} dx\;\left\{\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\;\varphi^*(k)e^{-ikx}\right\}\left\{\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk'\;\varphi(k')e^{ik'x}\right\} \\
&= \int_{-\infty}^{\infty} dk\;\int_{-\infty}^{\infty} dk'\;\varphi^*(k)\varphi(k')\;\frac{1}{2\pi}\;\int_{-\infty}^{\infty} dx\;e^{i(k'-k)x} \\
&= \int_{-\infty}^{\infty} dk\;\int_{-\infty}^{\infty} dk'\;\varphi^*(k)\varphi(k')\;\delta(k'-k) \;=\; \int_{-\infty}^{\infty} dk\;\varphi^*(k)\varphi(k) \\
&= \int_{-\infty}^{\infty} dk\;\left|\varphi(k)\right|^2 \;=\; 1 \quad .
\end{aligned} \tag{6}$$

Performing the integral of formula (1) for the Fourier transform (3) is straightforward as we see:

$$\begin{aligned}
\psi(x,t=0) \;&=\; \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\;\varphi(k)e^{ikx} \;=\; \frac{1}{2\sqrt{\pi\Delta k}}\int_{\bar{k}-\Delta k}^{\bar{k}+\Delta k} dk\;e^{ikx} \\
&= \frac{1}{2\sqrt{\pi\Delta k}}\;\frac{1}{ix}\left\{e^{i(\bar{k}+\Delta k)x}-e^{i(\bar{k}-\Delta k)x}\right\} \\
&= \frac{1}{\sqrt{\pi\Delta k}}\;e^{i\bar{k}x}\;\frac{\sin\left(\Delta k\; x\right)}{x} \quad ,
\end{aligned} \tag{7}$$

which is right the function given in formula (4).

Problem 1

Study the following expression for the probability distribution, $P(x, t = 0)$, of a particle along the x-axis at instant $t = 0$.

$$P(x, t = 0) \;=\; \frac{\sin^2(x)}{\pi x^2} \tag{8}$$

Determine $P(x = 0, t = 0)$ (remember $\sin(x) \approx x$ for small values of x).
Make a graphical representation of the probability distribution $P(x, t = 0)$ as a function of x and interpret your result.
What is the most probable x position for finding the particle?
What is the probability to find the particle at $x = 5000$?

Problem 2

Determine the integration of Eq. (1) for the distribution $\varphi(k)$ given by

$$\varphi(k) \;=\; \begin{cases} 1/\sqrt{2} & \text{for} \quad 0 \le k \le 2 \\ 0 & \text{for} \quad k < 0 \;\text{ and }\; k > 2 \end{cases} . \tag{9}$$

and compare the result with the probability distribution $P(x, t = 0)$ of Problem 1 (remember $P = |\psi|^2$).

Problem 3

Make a graphical representations of the probability distribution

$$P(x, t) \;=\; \frac{\sin^2(x - t)}{\pi (x - t)^2} \tag{10}$$

as a function of x for $t = 0$ (Problem 1), $t = 1$, $t = 2$ and $t = 3$, and interpret your result.

Problem 4

Imagine an experiment where at instant $t = 0$ we measure the position of a quantum particle. The experiment is 100 times repeated. The time starts counting everytime at the beginning of the experiment. One obtains the following result.

The particle is never found for $x < -4.5$, or for $x > 5.5$, 3 times in the interval $-4.5 < x < -3.5$, 1 time in the interval $-3.5 < x < -2.5$, 7 times in the interval $-2.5 < x < -1.5$, 20 times in the interval $-1.5 < x < -0.5$, 34 times in the interval $-0.5 < x < 0.5$, 24 times in the interval $0.5 < x < 1.5$, 8 times in the interval $1.5 < x < 2.5$, 0 times in the interval $2.5 < x < 3.5$, 2 times in the interval $3.5 < x < 4.5$ and 1 time in the interval $4.5 < x < 5.5$. Make a histogram for this experiment.

In the following we choose $x = 2$ for the position of the particle when it is found in the interval $1.5 < x < 2.5$ and similar for the particle's position in the other intervals. This way we may represent the experiment by

x	-4	-3	-2	-1	0	1	2	3	4	5
# times	3	1	7	20	34	24	8	0	2	1

Calculate the most probable value for the position of the particle at the instant $t = 0$.

1.1 Expectation value

For the most probable, or average, position, which was obtained in Problem 2, we obtained an expression of the form

$$< x > = \sum_x P(x, t = 0)\, x \quad . \tag{11}$$

The expression contains a sum because the x variable was divided up into finite intervals. In the following, as before, we consider x a continuous variable. The sum turns then into an integral

$$< x > = \int_{-\infty}^{+\infty} dx\, P(x, t = 0)\, x \quad . \tag{12}$$

Using Eq. (2), we may also write

$$< x > = \int_{-\infty}^{+\infty} dx\ |\psi(x, t = 0)|^2\ x \ = \int_{-\infty}^{+\infty} dx\ \{\psi(x, t = 0)\}^*\ x\ \ \psi(x, t = 0) \quad . \tag{13}$$

The symmetric final form on the righthand side of Eq. (13) is not completely innocent as we will see in the following sections. It is actually the precise definition of expectation values for operators in quantum mechanics.

In the case of the expectation value of the quantity x it does not make much difference whether we write first complex conjugate of the wave function, then the quantity x and finally the wave function itself, or some other order. But most other quantities are in quantum mechanics represented by differential and more complicated operators. In such cases the order really matters.

1.2 Momentum

In general a particle has velocity. So, we might wonder how velocity is represented by a wave packet. However, before studying the particle's dislocation in time we first determine its momentum. The time development of the wave packet we leave for a subsequent section.

The expectation value of momentum is in quantum mechanics defined by

$$\langle k \rangle \ = \int_{-\infty}^{\infty} dx\ \psi^*(x) \left\{ -i \frac{\partial}{\partial x} \right\} \psi(x) \quad . \tag{14}$$

For the example (4) we obtain for the above expression the result

$$\langle k \rangle \ = \ \bar{k} \quad . \tag{15}$$

The calculations can most easily be performed by following the same steps as in formula (6), *i.e.*

$$
\begin{aligned}
\langle k \rangle &= \int_{-\infty}^{\infty} dx\ \psi^*(x,t=0) \left\{ -i\frac{\partial}{\partial x} \right\} \psi(x,t=0) \\
&= \int_{-\infty}^{\infty} dx \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\ \varphi^*(k) e^{-ikx} \right\} \left\{ -i\frac{\partial}{\partial x} \right\} \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk'\ \varphi(k') e^{ik'x} \right\} \\
&= \int_{-\infty}^{\infty} dx \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\ \varphi^*(k) e^{-ikx} \right\} \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk'\ \varphi(k')\ k'\ e^{ik'x} \right\} \\
&= \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk'\ \varphi^*(k)\varphi(k')\ k'\ \frac{1}{2\pi} \int_{-\infty}^{\infty} dx\ e^{i(k'-k)x} \\
&= \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk'\ \varphi^*(k)\varphi(k')\ k'\ \delta(k'-k) \ = \ \int_{-\infty}^{\infty} dk\ \left|\varphi(k)\right|^2\ k \\
&= \int_{\bar{k}-\Delta k}^{\bar{k}+\Delta k} dk\ \frac{k}{2\Delta k} \ = \ \bar{k} \quad .
\end{aligned} \tag{16}
$$

We find thus that the most probable value to be measured for the particle's momentum, or the average value for a repeated number of measurements, equals $\bar{k}$ which is indeed the central value of the k-distribution. As a consequence of this result one interprets the integration variable k in the Fourier expansion defined in formula (1) as the *momentum* of the Fourier component in the expansion. This has then moreover as a consequence that the time development of each Fourier component is different and thus in general that the wave packet tends to spread.

1.3 The Heisenberg uncertainty relation

By describing the motion of a particle by a wave packet, one introduces some uncertainty in the particle's position as well as some uncertainty in the particle's momentum. For instance, in the previous example as well the momentum distribution (3) as the position distribution (4) have some spreading. From figure (1a) we learn that the uncertainty in the momentum of the particle equals Δk, *i.e.*

$$
k \ = \ \bar{k} \pm \Delta k \quad . \tag{17}
$$

Moreover, from figure (1b) we may estimate that the width of the probability distribution equals about $\pi/\Delta k$, which amounts for the uncertainty in the particle's position to

$$
\Delta x \ \approx \ \frac{\pi}{2\Delta k} \quad . \tag{18}
$$

Consequently, for the product of the two uncertainties we obtain

$$
\Delta k\ \Delta x \ \approx \ \tfrac{1}{2}\pi \ > \ \tfrac{1}{2} \quad , \tag{19}
$$

for which we recognize the Heisenberg relation in units $\hbar = 1$.

1.4 The time development of a wave packet

The general expression for the time development of a wave packet is as follows:

$$\psi(x,t) \; = \; \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \; \varphi(k) \exp\left\{ i \left(kx - \omega(k)t \right) \right\} \quad , \tag{20}$$

where $\omega(k)$ is some function of momentum k.

In order to study the above expression (20), we assume that ω is linear in k, at least for values where the Fourier transform φ is maximal, *i.e.*

$$\omega(k) \; = \; \bar{\omega} \; + \; \bar{\omega}'(k - \bar{k}) \quad . \tag{21}$$

Such choice for ω leads for the wave packet (20) to the expression

$$\begin{aligned}
\psi(x,t) \; &= \; \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \; \varphi(k) \exp\left\{ i \left(kx - \left[\bar{\omega} \; + \; \bar{\omega}'(k - \bar{k}) \right] t \right) \right\} \\
&= \; \frac{1}{\sqrt{2\pi}} \exp\left\{ i \left(-\bar{\omega}t + \bar{\omega}'\bar{k}t \right) \right\} \int_{-\infty}^{\infty} dk \; \varphi(k) \exp\left\{ ik \left(x - \bar{\omega}'t \right) \right\} \\
&= \; \exp\left\{ it \left(-\bar{\omega} + \bar{\omega}'\bar{k} \right) \right\} \; \psi(x - \bar{\omega}'t, 0) \quad ,
\end{aligned} \tag{22}$$

which implies that apart from a phase factor and a translation along the x-axis, the wave packet at the instant t has the same form as the wave packet at the instant $t = 0$. For the probability distribution one finds consequently

$$\left| \psi(x,t) \right|^2 \; = \; \left| \psi(x - \bar{\omega}'t, 0) \right|^2 \quad . \tag{23}$$

From the latter formula we read that the central peak in the probability distribution, which according to figure (1b) at $t = 0$ is found at the origin of the x-axis, is located at the position $x = \bar{\omega}'t$ at the instant of time t. Consequently, for ω linear in k as in formula (21), the wave packet moves with a constant velocity $\bar{\omega}'$ and hence represents a freely moving particle. The general idea is depicted in figure (2).

Notice, that for ω linear in k as in formula (21), the wave packet does not spread as time develops. A feature which at first sight also seems quite reasonable for a point particle in the absence of external forces. However, as we will see later on in subsection (1.6), in general ω is not linear in k as in formula (21). Hence, also quadratic and higher order terms must be considered which in general leads to spreading.

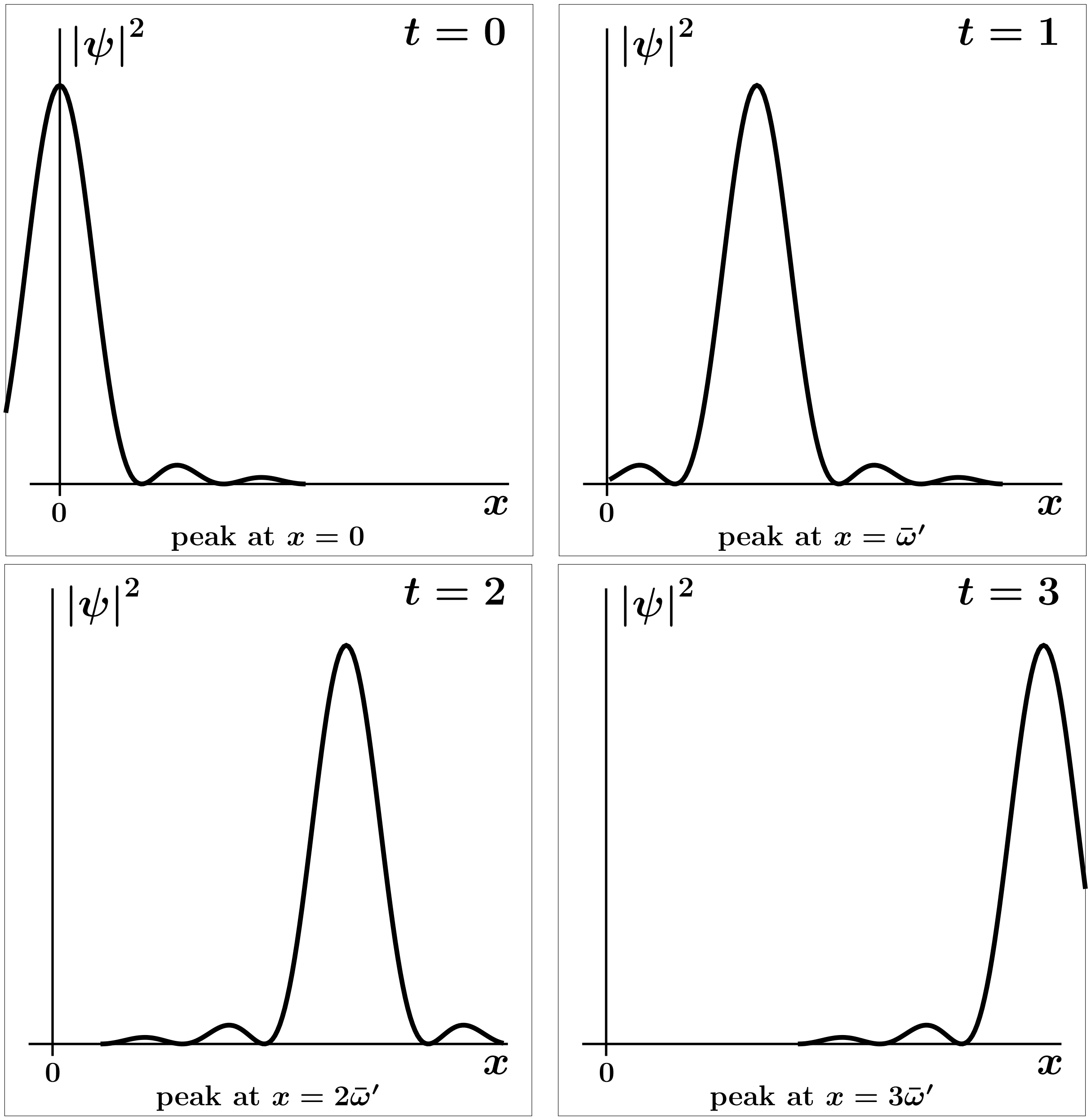


Figure 2: The probability distribution (23) in space (x) of wave packet (22) for the momentum distribution (3) at four different instances, $t = 0$, 1, 2 and 3. The position of the maximum probability, which represents the most probable place where the particle can be found, moves at constant velocity $\bar{\omega}'$.

1.5 Energy

The expectation value of energy is in quantum mechanics related to the wave function's time development, and hence defined by

$$\langle E\rangle \ = \ \int_{-\infty}^{\infty} dx\ \psi^{*}(x,t)\left\{ i\frac{\partial}{\partial t}\right\}\psi(x,t) \quad . \tag{24}$$

For the example (3) and moreover under the assumption that ω is linear in k as in formula (21), we obtain for the above expression the result

$$\langle E\rangle \ = \ \bar{\omega} \quad . \tag{25}$$

The calculations can most easily be performed by following the same steps as in formula (14), *i.e.*

$$\begin{aligned}
\langle E\rangle \ &= \ \int_{-\infty}^{\infty} dx\ \psi^{*}(x,t)\left\{ -i\frac{\partial}{\partial t}\right\}\psi(x,t) \\
&= \ \int_{-\infty}^{\infty} dk\ \int_{-\infty}^{\infty} dk'\ \varphi^{*}(k)\varphi(k')\ \omega(k')\ e^{i\,(\omega(k)\,-\,\omega(k'))\,t}\ \delta(k'-k) \\
&= \ \int_{-\infty}^{\infty} dk\ |\varphi(k)|^{2}\ \omega(k) \ = \ \int_{\bar{k}\,-\,\Delta k}^{\bar{k}\,+\,\Delta k} dk\ \frac{\bar{\omega}\ +\ \bar{\omega}'(k-\bar{k})}{2\Delta k} \ = \ \bar{\omega} \quad .
\end{aligned} \tag{26}$$

We find thus that the most probable value to be measured for the particle's energy, or the average value for a repeated number of measurements, equals $\bar{\omega}$, which is the central value for the momentum distribution (3), since from expression (21) one has

$$\omega(k=\bar{k}) \ = \ \bar{\omega} \quad .$$

1.6 Momentum, velocity and energy

In the previous subsections we obtained for the wave packet representation (20) of a point particle, in the approximation that ω is linear in k as in formula (21), the following three results: The expectation values for the particle's momentum and energy are given in formulas (14) and (24) by respectively $\bar{k}$ and $\bar{\omega} = \omega(\bar{k})$; whereas the particle's velocity is given by $\bar{\omega}'$. The latter quantity can more generally be written in the form (Taylor expansion coefficient):

$$\bar{\omega}' = \left(\frac{d\omega(k)}{dk}\right)_{k\,=\,\bar{k}} \quad . \tag{27}$$

Now, in nonrelativistic mechanics we have the following relations between velocity v, momentum p, kinetic energy K and the particle's rest mass:

$$p = mv \quad \text{and} \quad K = \frac{p^2}{2m} \quad . \tag{28}$$

In comparison, we would expect for the wave packet something similar. But, then we are dealing with distributions. Suppose, however, that the uncertainty in momentum is very small. In that case the variable k is for all Fourier components almost equal to its average or expectation value $\bar{k}$. The first of the two relations (28) would then translate into

$$\bar{\omega}' = \frac{\bar{k}}{m} \quad , \tag{29}$$

whereas for the second relation one would expect

$$E \approx E(\bar{k}) = \frac{\bar{k}^2}{2m} \quad . \tag{30}$$

This suggests that we may identify the time development function $\omega(k)$ defined in formula (20), with the energy variable $E(k)$ for each Fourier component. Formula (30) suggests then the choice

$$E(k) = \frac{k^2}{2m} \quad . \tag{31}$$

A Taylor series expansion around the central value $k = \bar{k}$ of the latter expression for the k-depence of the energy variable $E(k)$, gives us

$$\begin{aligned} E(k) = \omega(k) &= E(\bar{k}) + \left(\frac{dE}{dk}\right)_{k\,=\,\bar{k}}\left(k-\bar{k}\right) + \frac{1}{2}\left(\frac{d^2E}{dk^2}\right)_{k\,=\,\bar{k}}\left(k-\bar{k}\right)^2 + \cdots \\ &= \frac{\bar{k}^2}{2m} + \frac{\bar{k}}{m}\left(k-\bar{k}\right) + \frac{1}{2m}\left(k-\bar{k}\right)^2 \end{aligned} \tag{32}$$

The above expansion is complete, since the higher order derivatives vanish. We may moreover observe that in case $\Delta k \ll \bar{k}$ one has that the third term in (32) is indeed much smaller than the second term. Hence, the assumption (21) is correct for such cases.

By comparing formula (21) to formula (32) we find from the first term indeed relation (30) and from the second term relation (29). Consequently, we may conclude that for the kinematics of a classical point particle the choice (31) is perfect.

1.7 Wave equation

Once the k-dependence of the energy variable $\omega(k) = E(k)$ has been settled, the wave equation follows immediatly. When, for instance, we determine the first derivative in t for the wave packet (20), we find

$$i\,\frac{\partial}{\partial t}\,\psi(x,t) \;=\; \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\;\varphi(k)\;E(k)\;e^{i\,(kx\,-\,E(k)t)} \quad . \tag{33}$$

Similarly, when we determine its second derivative in x, we obtain

$$\frac{\partial^2}{\partial x^2}\,\psi(x,t) \;=\; \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\;\varphi(k)\;\left(-k^2\right)\;e^{i\,(kx\,-\,E(k)t)} \quad . \tag{34}$$

Consequently, from the k-dependence (31) for $E(k)$, we find for the wave packet (20) the wave equation

$$\begin{aligned} i\,\frac{\partial}{\partial t}\,\psi(x,t) \;&=\; \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\;\varphi(k)\;E(k)\;e^{i\,(kx\,-\,E(k)t)} \\ &=\; \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\;\varphi(k)\;\frac{k^2}{2m}\;e^{i\,(kx\,-\,E(k)t)} \\ &=\; -\frac{1}{2m}\,\frac{\partial^2}{\partial x^2}\,\psi(x,t) \quad , \end{aligned} \tag{35}$$

for which we recognize the Schrödinger equation in units $\hbar = 1$ for a system without interactions.

Notice, at this stage, that such wave equation just depends on our choice for the k-dependence for $E(k)$, in this case given by (31). Might we, for example, have preferred a k-dependence for $E(k)$ of the form

$$E(k) \;=\; \sqrt{k^2+m^2} \quad , \tag{36}$$

then we would have obtained for the wave equation of (20) the result

$$\begin{aligned} \frac{\partial^2}{\partial t^2}\,\psi(x,t) \;&=\; \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\;\varphi(k)\;\left(-E^2(k)\right)\;e^{i\,(kx\,-\,E(k)t)} \\ &=\; \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\;\varphi(k)\;\left(-k^2-m^2\right)\;e^{i\,(kx\,-\,E(k)t)} \\ &=\; \left(\frac{\partial^2}{\partial x^2}\;-\;m^2\right)\;\psi(x,t) \quad , \end{aligned} \tag{37}$$

for which we recognize the Klein-Gordon equation in units $\hbar = 1$ for a system without interactions.

Consequently, the wave packet description in itself does not say anything about the dynamics of the system. It is just a consistent way of describing quantum mechanically the motion of a particle.

1.8 Plane wave

In the limit of vanishing Δk, one obtains a particle with a very well defined momentum, *i.e.* $\bar{k}$, but with a constant and thus vanishing probability distribution along the x-axis as can be seen, for instance by using formula (4), *i.e.*

$$\frac{1}{\sqrt{\pi \Delta k}}\, e^{i\bar{k}x}\, \frac{\sin(\Delta k\; x)}{x} \quad \underset{\Delta k \to 0}{\longrightarrow} \quad \sqrt{\frac{\Delta k}{\pi}}\, e^{i\bar{k}x} \quad . \tag{38}$$

The image of a particle being everywhere with the same probability and with a well-defined momentum, applies well to a beam of particles. One speaks then of a *plane wave* which has the form:

$$\psi(x) \;=\; \frac{e^{i\bar{k}x}}{\sqrt{2\pi}} \quad . \tag{39}$$

The fact that a plane wave is not normalizable, can then be interpreted as describing the infinite number of particles in the beam.

2 Three dimensional wave packet

The generalization of the one dimensional wave packet (20) to three dimensions is straightforward. We define the position coordinates

$$x_1 \ , \ x_2 \ \text{and} \ x_3 \ , \tag{40}$$

and similarly the three components of momentum

$$k_1 \ , \ k_2 \ \text{and} \ k_3 \ . \tag{41}$$

and generalize wave packet (20) to a wave packet which describes a particle which moves in three dimensions by

$$\psi(\vec{x},t) \ = \ \left(\frac{1}{2\pi}\right)^{3/2} \int d^3k \, \varphi\left(\vec{k}\right) \exp\left\{ i \left[\vec{k} \cdot (\vec{x} - \vec{x}_0) - E\left(\vec{k}\right) t \right] \right\} \quad , \tag{42}$$

where $\vec{x}_0$ represents the "position" of the particle at $t = 0$.

2.1 Example

Let us study here the generalization to three dimensions of a Fourier transform φ which only differs appreciably from zero in a small area of momentum space surrounding a central value $\vec{\bar{k}}$, *i.e.* a wave packet which represents a particle with "momentum" $\vec{\bar{k}}$. In practice we will study the generalization of example (3), given by

$$\begin{aligned} \varphi(k) \ &= \ \prod_{i=1}^{3} \frac{1}{\sqrt{2\Delta k_i}} \ \theta\left(\left(k_i - \bar{k}_i\right)^2 - \left(\Delta k_i\right)^2 \right) \qquad (43) \\ &= \ \begin{cases} \dfrac{1}{2\sqrt{2\Delta k_1 \Delta k_2 \Delta k_3}} & , \left|k_i - \bar{k}_i\right| \leq \Delta k_i \quad i = 1, \ \text{and} \ \ i = 2, \ \ \text{and} \ \ i = 3 \\ 0 & , \left|k_i - \bar{k}_i\right| > \Delta k_i \quad i = 1, \ \text{or} \ \ i = 2, \ \ \text{or} \ \ i = 3 \end{cases} \end{aligned}$$

It represents a function $\varphi\left(\vec{k}\right)$ which vanishes everywhere in momentum space, except for the interior of a box with sides of length $2\Delta k_1$, $2\Delta k_2$ and $2\Delta k_3$ centered at $\vec{\bar{k}}$.

The wave packet ψ, which according to equation (42) follows at the instant $t = 0$ for the above choice (43) of Fourier transform φ, can, by performing three times the same integration as shown in formula (7), readily be determined to be given by

$$\psi(\vec{x}, t = 0) \ = \ e^{i\vec{\bar{k}} \cdot (\vec{x} - \vec{x}_0)} \prod_{i=1}^{3} \frac{1}{\sqrt{\pi \Delta k_i}} \ \frac{\sin\left(\Delta k_i \ \left[x_i - (\vec{x}_0)_i\right]\right)}{x_i - (\vec{x}_0)_i} \quad , \tag{44}$$

the probability distribution of which expression has a large maximum centered around $\vec{x}_0$ as in the three dimensional generalization of figure (1b).

2.2 Velocity and wave equation

Let us suppose that for a classical particle in three dimensions serves the generalization of the k-dependence for the energy E in one dimension as given in formula (31), i.e.

$$E\left(\vec{k}\right) = \frac{\vec{k}^{\,2}}{2m} \tag{45}$$

A Taylor series expansion of this expression around the central value $\vec{\bar{k}}$ gives us

$$\begin{aligned} E\left(\vec{k}\right) &= E(\vec{\bar{k}}) + \sum_{i=1}^{3}\left(\frac{\partial E}{\partial k_i}\right)_{\vec{k}=\vec{\bar{k}}}\left(k_i - \bar{k}_i\right) + \cdots \\ &= \frac{\vec{\bar{k}}^{\,2}}{2m} + \frac{\vec{\bar{k}}}{m}\cdot\left(\vec{k} - \vec{\bar{k}}\right) + \cdots \end{aligned} \tag{46}$$

When we restrict ourselves to the first two terms of this expansion, which for small values of Δk_1, Δk_2 and Δk_3 leads to a very good approximation, then we obtain, following a similar calculus as in formula (22), for the probability distribution in coordinate space at the instant t the result

$$\left|\psi\left(\vec{x},t\right)\right|^2 = \left|\psi\left(\vec{x} - \frac{\vec{\bar{k}}}{m}t, 0\right)\right|^2 \quad . \tag{47}$$

From the latter formula we read that the central peak in the probability distribution, which at $t = 0$ is found at the position $\vec{x}_0$, is located at the position $\vec{x} = \vec{x}_0 + \frac{\vec{\bar{k}}}{m}t$ at the instant of time t. Consequently, the wave packet moves with a constant velocity $\frac{\vec{\bar{k}}}{m}$ and hence represents a freely moving particle in three dimensions.

The *wave equation* which follows for the k-dependence of the energy given in formula (45), can be determined by a procedure similar to the one discussed in section (1.7), and yields

$$i\frac{\partial}{\partial t}\psi\left(\vec{r},t\right) = -\frac{\nabla^2}{2m}\psi\left(\vec{r},t\right) \quad \text{where} \quad \nabla^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} \quad , \tag{48}$$

for which one recognizes the three dimensional Schrödinger equation for a system without interactions.