Gaussian wave packet

The Gaussian wave function is determined by its wave function in the wave-vector space. In 1-dimensional space it is:

\[ f(k) = A \exp\left(\frac{-(k-k_0)^2}{4\Delta_k^2}\right), \tag{1} \]

where \( A \) is the normalization constant and \( \Delta_k \) is the width of the packet in the \( k \)-space. Its graph as function of \( K \) is a bell-shaped curve centered near \( k_0 \). The normalization constant should be found from the normalization condition \( \int_{-\infty}^{\infty} |f(k)|^2 \, dk = 1 \). This integral is of the Gaussian type. Gaussian integral in 1 dimension is defined reads:

\[ I(\alpha) = \int_{-\infty}^{\infty} \exp\left(-\alpha x^2\right) \, dx = \sqrt{\frac{\pi}{\alpha}} \tag{2} \]

Employing this formula one finds \( A = (2\pi)^{-1/4}\Delta_k^{-1/2} \). To relate \( \Delta_k \) to the average characteristics of the Gaussian wave packet, let us calculate the average square of the deviation of the wave vector from its central point \( k = k_0 \) (quantum fluctuation or square of uncertainty). Its definition is:

\[ \langle (\Delta k)^2 \rangle = \int_{-\infty}^{\infty} (k-k_0)^2 \, |f(k)|^2 \, dk \tag{3} \]

This integral is reduced to the integral of a type:

\[ I_1(\alpha) = \int_{-\infty}^{\infty} x^2 \exp\left(-\alpha x^2\right) \, dx = -\frac{dI}{d\alpha} = \frac{I(\alpha)}{2\alpha} \tag{4} \]

Employing this equation, we find that \( \langle (\Delta k)^2 \rangle = \Delta_k^2 \).

Next we find the wave function of the Gaussian packet in the coordinate space applying the standard Fourier transformation:

\[ \psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(k) e^{ikx} \, dk \tag{5} \]

This integral is reduced to a slightly generalized standard Gaussian integral (2):

\[ I(\alpha, \beta) = \int_{-\infty}^{\infty} \exp\left(-\alpha x^2 + i\beta x\right) \, dx = \sqrt{\frac{\pi}{\alpha}} \exp\left(\frac{\beta^2}{2\alpha}\right) \tag{6} \]

Employing the latter equation with \( \alpha = 1/(4\Delta_k^2) \) and \( \beta = ix \) eq. (1) for \( f(k) \), one can transform eq. (5) as follows:

\[ \psi(x) = \frac{e^{ik_0 x} \sqrt{\Delta_k}}{\sqrt{\pi}} \exp\left(-\Delta_k^2 x^2\right) \tag{7} \]
This wave function has the shape of the Gaussian wave packet (2), but in the coordinate space. It is centered at \( x = 0 \) and its width is \( \Delta_x = 1/(2\Delta k) \). The wave function

\[
\psi(x) = (2\pi)^{-1/4} \Delta_x^{-1/2} \exp \left( -\frac{x^2}{4\Delta^2_x} \right)
\]

is automatically normalized as it follows from Percival theorem. We also find the uncertainty relation in the form \( \Delta_x \Delta_k = 1/2 \). We will see that at any non-zero time \( t > 0 \) the coordinate uncertainty increases.

To find the time evolution of the Gaussian wave packet we again start with the wave function in the \( k \)-space, since the energy is well defined for the states with fixed \( k \): \( E(k) = \frac{\hbar^2 k^2}{2m} \). Thus, the time evolution of the wave function (1) has the following form:

\[
f(k, t) = (2\pi)^{-1/4} \Delta_k^{-1/2} \exp \left[ \frac{-(k - k_0)^2}{4\Delta^2_k} - \frac{i\hbar k^2 t}{2m} \right]
\]

The modulus of this wave function does not depend on time since the modulus of the factor \( \exp \left( \frac{-i\hbar k^2}{2m} \right) \) is 1. Thus, the average square of the momentum fluctuation is the same as at \( t = 0 \) (equal to \( \Delta^2_k \)). However, the uncertainty of coordinate increases with time as it is shown below. The time dependent wave function \( \psi(x, t) \) is the Fourier transform of the function \( f(k, t) \) (9):

\[
\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(k, t) e^{ikx} dk
\]

The integral is again of the Gaussian type (6). The exponential integrand has the argument

\[
-\frac{(k - k_0)^2}{4\Delta^2_k} + ikx - \frac{i\hbar k^2 t}{2m}
\]

It is reasonable to subtract from it its value at \( k = k_0 \) and compensate it by a factor \( \exp \left( i k_0 x - \frac{i\hbar k^2 t}{2m} \right) \) in front of the integral. Then the exponent in the integrand acquires a form:

\[
-\frac{(k - k_0)^2}{4\Delta^2_k} + i(k - k_0)x - \frac{i\hbar (k^2 - k_0^2)}{2m}
\]

The last term can be transformed using a simple identity \( k^2 - k_0^2 = (k - k_0)^2 + 2k_0 (k - k_0) \). Then the previous expression for the argument (11) can be rewritten as follows:

\[
-\left( \frac{1}{4\Delta^2_k} + \frac{i\hbar}{2m} \right) (k - k_0)^2 + i (k - k_0) (x - v_0 t)
\]

where \( v_0 = \hbar k_0/m \) is the classical velocity of the center of the packet. It is also reasonable to replace in the previous expression the fraction \( \frac{1}{4\Delta^2_k} \) by \( \Delta^2_x \). Then
the integral is exactly the Gaussian $I(\alpha, \beta)$ (6) with $\alpha = \Delta^2_x + i\hbar t/(2m)$ and $\beta = x - v_0 t$. Thus, we find:

$$\psi(x, t) = \frac{\exp \left[ i k_0 x - \frac{i \hbar k_0^2 t}{2m} - \frac{(x - v_0 t)^2}{4(\Delta^2_x + \frac{\hbar t}{2m})} \right]}{(2\pi)^{1/4} \left( \Delta^2_x + \frac{i\hbar t}{2m} \right)^{1/2}}$$

(12)

Its square of modulus reads:

$$|\psi(x, t)|^2 = \frac{\exp \left[ -\frac{(x - v_0 t)^2}{2(\Delta x(t))^2} \right]}{\sqrt{2\pi} \Delta x(t)}$$

(13)

where $\Delta x(t) = \left( \Delta^2_x + \frac{\hbar^2 t^2}{4m^2 \Delta^2_x} \right)^{1/2}$ is the time-dependent uncertainty of the particle coordinate. We see that it remains practically unchanged at $t \ll t_0 = \frac{2m \Delta^2_x}{\hbar}$. Asymptotically at $t \gg t_0$, the uncertainty of coordinate grows linearly with time: $\frac{\Delta x(t)}{\Delta x} \approx \frac{t}{t_0}$. The wave packet smears out with time since it is a superposition of states with different velocities. It is easy to estimate the uncertainty of velocity $\Delta v = \hbar \Delta k / m$. At sufficiently large time it leads to the smearing of the wave packet to the width $\Delta x(t) \sim \Delta v t \sim \frac{\hbar \Delta k}{m} t \sim \frac{\hbar^2}{\pi \Delta x}$. This expression coincides with the asymptotic obtained from exact solution, but this estimate has more general character and relates to any wave packet. It is valid when the packet smearing due to the dispersion of velocity becomes larger than the initial width of the wave packet $\Delta x$, i.e. at $t > t_0$. 