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Analysis of the spreading Gaussian wave packet

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Abstract

The $\psi(x,t)$ wave function of a Gaussian wave packet spreading in free space ($V(x) \equiv 0$) is expressed in a didactic form. The expression found is a product of pure real factors and pure phase factors. This makes very easy to derive the expression for the probability density from the wave function. The physical meaning of each of the factors is analysed.

INTRODUCTION

While writing a paper [1] about the time evolution of different wave packets I wanted to find a didactic expression for the $\psi(x,t)$ wave function of a *Gaussian* initial state. The particular expression that was constructed at last is different from the ones found in quantum mechanics texts [2,3].

INITIAL STATE

Our initial state is a simple *Gaussian* wave packet of the form:

$$\psi_0(x; a, x_0, p_0) = \sqrt[4]{\frac{2}{\pi a^2}} \cdot \exp\left(i\frac{p_0}{\hbar}x\right) \cdot \exp\left(-\frac{(x-x_0)^2}{a^2}\right). \tag{1}$$

This wave packet is a product of three factors:

- A normalisation factor that makes the norm $\int_{-\infty}^{+\infty} |\psi(x)|^2 dx$ of the wave function to be unity.
- A plane wave factor that accounts for the non zero momentum p_0 of the wave packet.
- A bell-shaped localising function with half width at half maximum $\sqrt{\ln 2} \cdot a$.

TIME EVOLUTION

The time development of the initial $\psi_0(x)$ state is given by [2]:

$$\psi(x,t) = \mathcal{F}^{-1}\left[\mathrm{g}(k)\exp\left(-i\frac{k^2}{2}t\right)\right](x) \tag{2}$$

$$\mathrm{g}(k) = \mathcal{F}\left[\psi_0(x)\right](k) \tag{3}$$

This *Fourier integral* can be calculated easily with Gaussian integrals and leads to a wave function like this:

$$\psi(x,t) = \sqrt[4]{\frac{2}{\pi a^2(1+2i\cdot\hbar/m\cdot t/a^2)^2}} \exp\left(\frac{-(x-x_0)^2 - 2p_0/m\cdot x_0 t + ia^2\cdot p_0/\hbar\cdot x - ia^2\cdot p_0^2/(2m)/\hbar\cdot t}{a^2(1+2i\cdot\hbar/m\cdot t/a^2)}\right) \tag{4}$$

TRANSFORMATION OF $\psi(x,t)$ INTO DIDACTIC FORM

Now we want to transform this into something more informative. First note that the center of the wave packet is moving with the *group velocity* $u_g = p_0/m$. Hence it is worth to write $x_0 + p_0/m \cdot t$ instead of x_0 into the first term of the numerator in the exponential. Working this out gives the following result:

$$\psi(x,t) = \sqrt[4]{\frac{2}{\pi a^2 (1 + 2i \cdot \hbar/m \cdot t/a^2)^2}} \tag{5}$$
$$\exp\left(-\frac{[x - (x_0 + p_0/m \cdot t)]^2}{a^2(1 + 2i \cdot \hbar/m \cdot t/a^2)}\right) \cdot \exp\left(i\frac{p_0}{\hbar}x\right) \cdot \exp\left(-i\frac{p_0^2}{2m}\frac{1}{\hbar}t\right)$$

It is getting clearer already! Now let's get rid of the complex denominators!

$$\frac{1}{1 + 2i \cdot \hbar/m \cdot t/a^2} = \frac{1 - 2i \cdot \hbar/m \cdot t/a^2}{1 + 4 \cdot \hbar^2/m^2 \cdot t^2/a^4} \tag{6}$$

Utilising this we get finally

$$\psi(x,t) = \sqrt[4]{\frac{2}{\pi |a(t)|^2}} \cdot \exp\left(-\frac{[x - (x_0 + p_0/m \cdot t)]^2}{|a(t)|^2}\right) \cdot \exp\left(i\frac{p_0}{\hbar}x\right) \tag{7}$$
$$\exp\left(2i\frac{\hbar}{m}\frac{t}{a^2}\frac{[x - (x_0 + p_0/m \cdot t)]^2}{|a(t)|^2}\right) \tag{8}$$
$$\exp\left(-\frac{i}{2}\arg a(t)\right) \cdot \exp\left(-i\frac{p_0^2}{2m}\frac{1}{\hbar}t\right) \tag{9}$$
$$a(t) = a + 2i\frac{\hbar}{m}\frac{t}{a} \tag{10}$$

where $\arg z$ is the phase of the complex number z, i.e. $\arg Re^{i\varphi} = \varphi$. Our $\psi(x,t)$ has three main factors (7, 8 and 9). The first factor (7) is a product of two *pure real* coefficients and a plane wave. This plane wave part of *factor 1.* and the entire second (8) and third (9) factors are pure *phase factors*, i.e. their magnitude is one. Hence it is very easy to calculate the probability density $\rho(x,t) = |\psi(x,t)|^2$: one has only to calculate the square of the pure real coefficients of *factor 1.* which gives:

$$\rho(x,t) = \sqrt{\frac{2}{\pi |a(t)|^2}} \exp\left(-2\,\frac{[x - (x_0 + p_0/m \cdot t)]^2}{|a(t)|^2}\right) \tag{11}$$

The three terms of $\psi(x,t)$ are as follows:

Factor 1. (Cf. 7.) A Gaussian of the form (1). This is an expression having the same form as $\psi_0(x)$ but the center of gravity of the Gaussian is moving with speed $u_g = p_0/m$ and its width is increased to $|a(t)| = \sqrt{a^2 + 4 \cdot \hbar^2/m^2 \cdot t^2/a^2}$. The maximum value of the Gaussian is decreasing as its width increases making the area under $\rho(x,t)$ (total probability) constant (one). Time evolution of *Factor 1* is shown in *Fig 1/a.*

Factor 2. (Cf. 8.) An x and t dependent phase factor that is quadratic in x. One can see from *Fig 1/b* that this factor oscillates faster for larger $|x|$ values. This accounts for the fact that the higher momentum components of the initial Gaussian $\psi_0(x)$ move with higher velocities. The function which describes the time dependent prefactor of the phase is $2 \cdot t/\left(a \cdot |a(t)|\right)^2$. This function (Cf. *Fig 2/a*) is not monotonic in time. Its value is zero for $t = 0$ and $t = \infty$ and has a maximum at $t = m/\hbar \cdot a^2/2$.

Factor 3. (Cf. 9.) An x independent (but still t dependent) phase factor. This phase factor is a product of two terms. The first term is a monotonic function of time while the second one is oscillating. The phase of the first term is zero for $t = 0$ ($a(t)$ is pure real) and $-\pi/4$ for $t = \infty$ ($a(t)$ is pure imaginary). The second term is $\exp(-i\omega_0 t)$ where $\omega_0 = E/\hbar = p_0^2/(2m)/\hbar$ and it accounts for the time development of the plane wave component $\exp(ip_0/\hbar \cdot x)$ in *Factor 1.* These two phase factors are plotted in *Fig 2/b, 2/c* against time.

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REFERENCES

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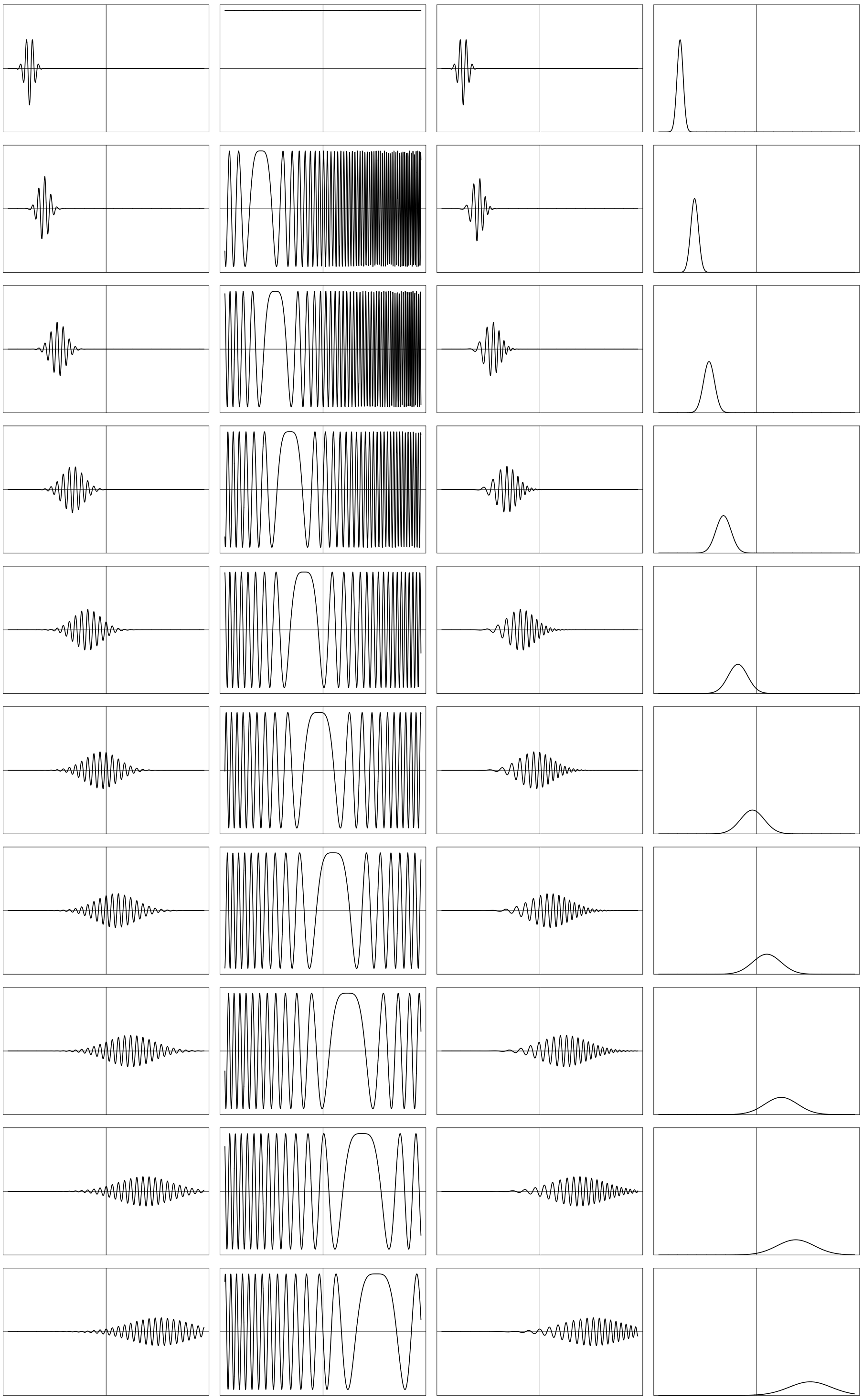

FIG. 1: x and t dependent parts of the wave function. Figs **a, b** and **c** show the time development of the real part of *factor 1*, *factor 2* and of the full $\psi(x,t)$. The x, y scale is the same for all **a, b** and **c** figures. Fig **d** shows the time development of the probability density $\rho(x,t)$. The x, y scale is the same for all time instants. *Atomic units* ($\hbar = m_e = 1$) are used. $a = 2.5 Bohr = 0.13 nm$, $\lambda = h/p_0 = 8/3\, Bohr = 0.14 nm$. The atomic time unit is $2.41 \cdot 10^{-17} s$. See the text for details.

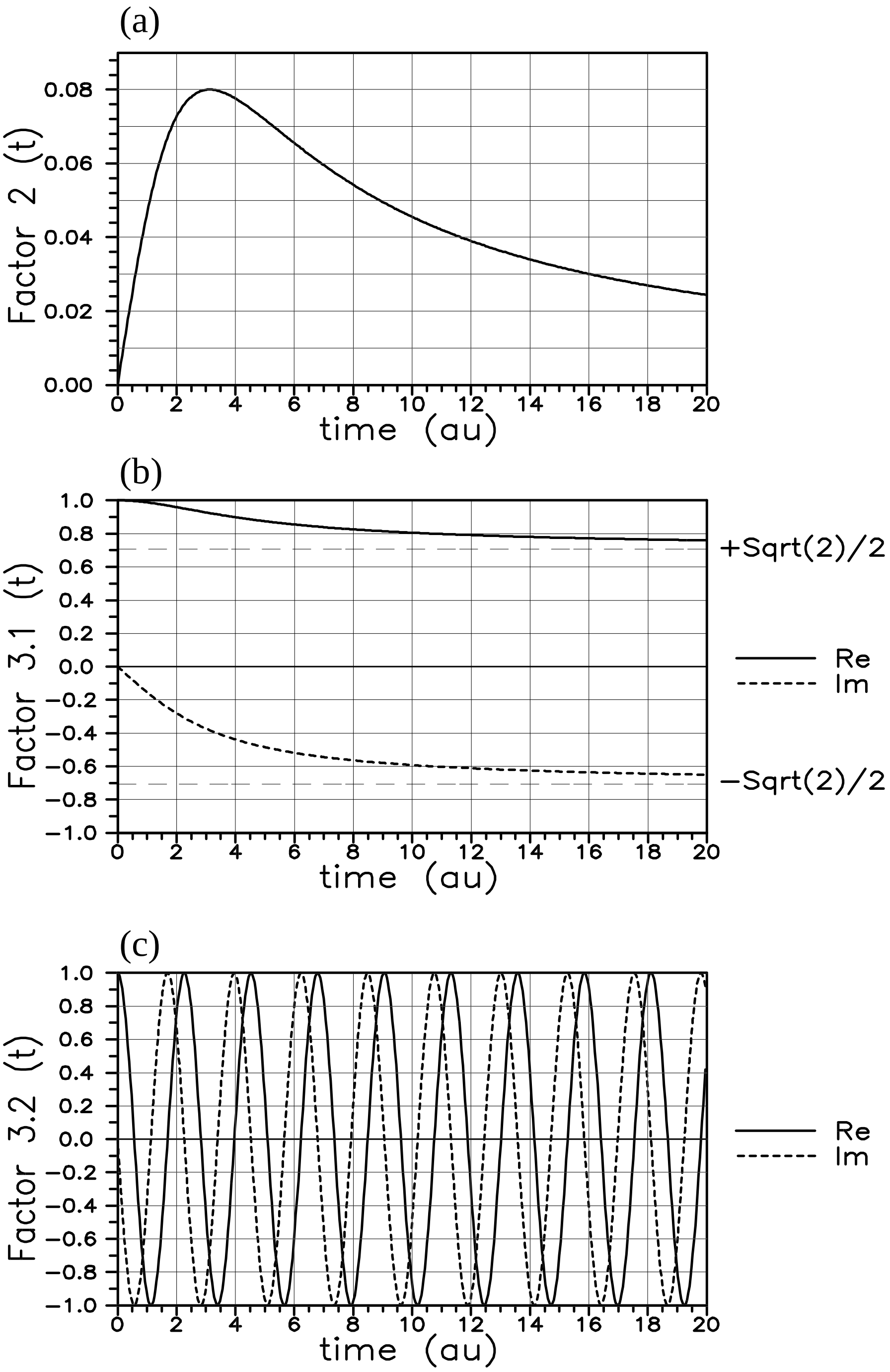

FIG. 2: t dependent parts of the wave function. Fig **a** shows the time dependent prefactor of *factor 2* as function of time. Figs **b** and **c** show the time dependence of the terms of *factor 3*. Their real (solid lines) and imaginary (dashed lines) parts are plotted against time. The thin dashed lines in Fig **b** show the asymptotes for $t = \infty$. *Atomic units* ($\hbar = m_e = 1$) are used. See the text for details.