# Propagation of a wave packet in a dispersive and dissipative medium

**Marcello Colozzo**

**Abstract**

The propagation of a wave packet in a dispersive and dissipative medium is really complicated (for a rigorous treatment we refer to [1]). We limit ourselves to an analysis deriving from series expansions truncated to the first order. We will start from a one-dimensional De Broglie wave packet relating to two special cases: 1) free particle; 2) particle in a periodic potential. In these two cases we will refute the assertion according to which the energy is transported with the group velocity, since the observable energy is not defined (the wave packet is a superposition of eigenfunctions of the energy). We will show however that the expectation value of the energy is transported with the group velocity.

The conclusions can be immediately generalized to the propagation of a packet of electromagnetic waves in a dispersive and dissipative medium, justifying the expression *group delay* of a wave packet.

## 1 Non-relativistic one-dimensional quantum system

Sia $S_q$ be a quantum system consisting of a particle of mass $m$ constrained to move on the $x$-axis, and subjected to a force field of potential energy $V(x)$, for which the Hamiltonian operator is with obvious meaning of the symbols:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \tag{1}$$

In particular, we consider the case where the spectrum $\sigma\left(\hat{H}\right)$ is purely continuous: $\sigma\left(\hat{H}\right) = \sigma_c\left(\hat{H}\right)$ or at most given by the union of continuous intervals separated by gaps. So that the eigenket system of the energy $\{|E\rangle\}$

$$\hat{H}|E\rangle = E|E\rangle$$

is a complete orthonormal system in the Hilbert space $\mathcal{H}$ associated with the system:

$$\int_{\sigma_c\left(\hat{H}\right)} dE\,|E\rangle\langle E| = \hat{1}, \quad \langle E|E'\rangle = \delta\left(E - E'\right) \tag{2}$$

Suppose that the initial state is a superposition of energy eigenstates; that is, $t = 0$:

$$|\psi_0\rangle = \int_{\sigma_c\left(\hat{H}\right)} dE\,|E\rangle\langle E|\psi_0\rangle \tag{3}$$

Let $c^{(0)}(E) = \langle E|\psi_0\rangle$, and taking into account the completeness relation of the eigenket system of the position $\{|x\rangle\}$:

$$\int_{-\infty}^{+\infty} dx\,|x\rangle\langle x| = \hat{1},$$

we have

$$c^{(0)}(E) = \langle E|\left(\int_{-\infty}^{+\infty} dx\,|x\rangle\langle x|\right)|\psi_0\rangle = \int_{-\infty}^{+\infty} dx\,\langle E|x\rangle\langle x|\psi_0\rangle$$

$\langle x|\psi_0\rangle = \psi_0(x)$ is the initial state ket in the coordinate representation, i.e. the initial wave function, while $\langle E|x\rangle = \langle x|E\rangle^* = u_E^*(x)$ where $u_E(x)$ is the eigenfunction of the energy corresponding to the eigenvalue $E$. Therefore: $c^{(0)}(E) = \int_{-\infty}^{+\infty} \psi_0(x)\,u_E^*(x)\,dx$. Writing (3) in the coordinate representation, we get $\psi_0(x) = \int_{\sigma_c\left(\hat{H}\right)} c^{(0)}(E)\,u_E(x)\,dE$.

So

$$\psi_0(x) = \int_{\sigma_c(\hat{H})} c^{(0)}(E) u_E(x) dE \tag{4}$$

$$c^{(0)}(E) = \int_{-\infty}^{+\infty} \psi_0(x) u_E^*(x) dx$$

which remind us of the Fourier transform.

## 2 Law of dispersion. Group velocity. Scattering

Incidentally, there is a class of quantum systems (free particle, particle in a periodic potential) for which $E = E(k)$ with $k \in (-\infty, +\infty)$, where for the free particle it is $k = p/\hbar$ where $p$ is the momentum, while in the case of the periodic potential $\hbar k$ is the crystalline momentum. In the case of the free particle the energy eigenfunctions are written (leaving aside the normalization factor)

$$u_k(x) = e^{ikx} \tag{5}$$

while for the periodic potential they are *Bloch waves* i.e. plane waves modulated in amplitude whose envelope is a periodic function with the same period as the potential. In both cases these are improper eigenfunctions since they are not elements of $\mathcal{L}^2(\mathbb{R})$. For simplicity we approximate the Bloch waves to (5). For the aforementioned class of systems the (4) become

$$\psi_0(x) = \int_{-\infty}^{+\infty} A(k) e^{ikx} dk \tag{6}$$

$$A(k) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \psi_0(x) e^{-ikx} dx$$

from which we see that $A(k) \overset{def}{=} c^{(0)}(E(k))$ is the Fourier transform[1] of $\psi_0(x)$. In accordance with the intuitive concept of particle, we assume as the initial profile of the wave function, a sinusoidal oscillation enveloped by a Gaussian:

$$\psi_0(x) = \sqrt{\frac{\alpha}{\sqrt{\pi}}} e^{-\frac{\alpha^2}{2}(x-x_0)^2} e^{ik_0(x-x_0)} \tag{7}$$

where $\alpha > 0$ and the wave number $k_0 \in \mathbb{R}$ are assigned. In the following calculations we will use the following notable integrals $(a > 0)$:

$$\int_{-\infty}^{+\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}} \tag{8}$$

$$\int_{-\infty}^{+\infty} x^2 e^{-ax^2} dx = \frac{1}{2}\sqrt{\frac{\pi}{a^3}}$$

$$\int_{-\infty}^{+\infty} e^{-ax^2+bx} dx = \sqrt{\frac{\pi}{a}} e^{-\frac{b^2}{4a}}$$

So the probability density

$$\rho_0(x) = \frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2(x-x_0)^2}$$

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[1] We have inserted the factor $\frac{1}{2\pi}$ because we have omitted the normalization factor in (5).

is a Gaussian distribution centered at $x_0$ and it is normalized:

$$\rho_0\left(x\right) = \left|\psi_0\left(x\right)\right|^2, \quad \int_{-\infty}^{+\infty} \rho_0\left(x\right)dx = 1$$

The width of the distribution is the mean square deviation, which in quantum mechanics is called the *dispersion* of the observable. $x$:

$$\left(\Delta x\right)_{t=0} = \left\langle\left(x-x_0\right)^2\right\rangle^{1/2} = \left[\int_{-\infty}^{+\infty}\left(x-x_0\right)^2\rho_0\left(x\right)\right]^{1/2}$$

$$= \left[\frac{\alpha}{\sqrt{\pi}}\int_{-\infty}^{+\infty}\left(x-x_0\right)^2 e^{-\alpha^2\left(x-x_0\right)^2}\right]^{1/2}$$

But

$$\int_{-\infty}^{+\infty}\left(x-x_0\right)^2 e^{-\alpha^2\left(x-x_0\right)^2} \underset{y=x-x_0}{=} \int_{-\infty}^{+\infty} y^2 e^{-\alpha^2 y^2}dy = \frac{1}{2}\frac{\sqrt{\pi}}{\alpha^3}$$

i.e.

$$\left(\Delta x\right)_{t=0} = \frac{1}{\alpha\sqrt{2}}$$

Thus the dispersion of the observable position in the initial state $\psi_0\left(x\right)$ decreases as a increases. $\alpha$. In Fig. 1 we report the behavior of $\mathrm{Re}\,\psi_0\left(x\right)$.
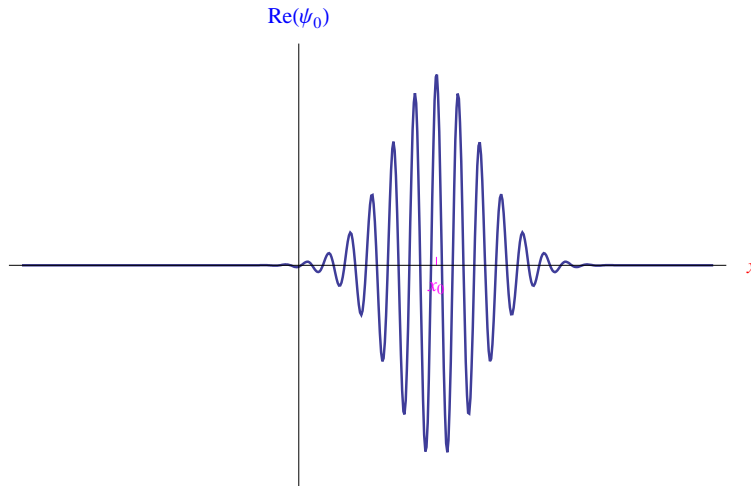


Figure 1: Trend of $\mathrm{Re}\,\psi_0\left(x\right)$.

Let's determine $A(k)$:

$$
\begin{aligned}
A(k) &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \psi_0(x) e^{-ikx} dx \\
&= \frac{1}{2\pi} \sqrt{\frac{\alpha}{\sqrt{\pi}}} \int_{-\infty}^{+\infty} e^{-\frac{\alpha^2}{2}(x-x_0)^2} e^{ik_0(x-x_0)} e^{-ikx} dx \\
&= \frac{1}{2\pi} \sqrt{\frac{\alpha}{\sqrt{\pi}}} \int_{-\infty}^{+\infty} \exp\left[ -\frac{\alpha^2}{2}(x-x_0)^2 + ik_0(x-x_0) - ik(x-x_0) \right] dx \\
&= \frac{1}{2\pi} \sqrt{\frac{\alpha}{\sqrt{\pi}}} e^{-ikx_0} \int_{-\infty}^{+\infty} \exp\left[ -\frac{\alpha^2}{2}(x-x_0)^2 \underbrace{-i(k-k_0)(x-x_0)}_{=b} \right] dx \\
&= \frac{1}{2\pi} \sqrt{\frac{\alpha}{\sqrt{\pi}}} e^{-ikx_0} \frac{\sqrt{\pi}}{\alpha} e^{-\frac{(k-k_0)}{4\alpha^2}}
\end{aligned}
$$

In the last step we used the third of the (8). Finally:

$$
A(k) = \frac{\sqrt{\pi}}{2\alpha\pi} e^{-\frac{(k-k_0)}{4\alpha^2}} e^{-ikx_0} \tag{9}
$$

from which we see that $|A(k)|^2$ is a Gassian distribution centered at $k_0$, and with width proportional to $\alpha$. This result does not surprise us because it is a property of Gaussian distributions that are invariant under the Fourier transform, with widths in inverse proportion. More precisely, for $\alpha$ sufficiently small, the $|A(k)|^2$ is extremely peaked around $k_0$, so that the dominant contribution to $\psi_0(x)$ comes from the monochromatic components of wavenumber $k \in (k_0 - \Delta k, k_0 + \Delta k)$ with $\frac{\Delta k}{|k_0|} \ll 1$.

Applying the time evolution operator to the initial state $\psi_0(x)$:

$$
\psi(x,t) = \int_{-\infty}^{+\infty} A(k) e^{i(kx - \omega(k)t)} dk \tag{10}
$$

where $\omega(k) = \frac{E(k)}{\hbar}$, which defines the dispersion law. Precisely:

$$
\omega(k) = \begin{cases} \frac{\hbar k^2}{2m}, & V(x) = 0 \\ \text{periodic function of period } \frac{2\pi}{a}, & \text{where } a \text{ is the period of } V(x) \end{cases}
$$

If $\omega(k)$ it does not vary rapidly, taking into account that $A(k)$ is strongly peaked around $k_0$, we can develop $\omega(k)$ in power series around $k_0$, truncating the development at the end of the first order:

$$
\omega(k) = \omega_0 + v_g(k - k_0) \tag{11}
$$

where

$$
\omega_0 = \omega(k_0), \quad v_g = \left. \frac{d\omega(k)}{dk} \right|_{k=k_0} \tag{12}
$$

Replacing (12) in (10)

$$
\begin{aligned}
\psi(x,t) &= \int_{-\infty}^{+\infty} A(k) \exp\{kx - [\omega_0 + v_g(k - k_0)]t\} dk \\
&= \int_{-\infty}^{+\infty} A(k) \exp(kx - \omega_0 t - v_g tk + v_g tk_0) dk \\
&= \int_{-\infty}^{+\infty} A(k) e^{ik(x - v_g t)} e^{-i(\omega_0 - v_g k_0)t} dk
\end{aligned}
$$

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So

$$\psi(x,t) = e^{i(k_0 v_g - \omega_0)t} \int_{-\infty}^{+\infty} A(k) e^{ik(x - v_g t)} dk$$

Taking into account the first of the (6)

$$\int_{-\infty}^{+\infty} A(k) e^{ik(x - v_g t)} dk = \psi_0(x - v_g t)$$

so

$$\psi(x,t) = e^{i\Omega_0 t} \psi_0(x - v_g t) \tag{13}$$

where

$$\Omega_0 = k_0 v_g - \omega_0 \tag{14}$$

From (13) we see that the wave packet translates rigidly and uniformly with velocity $v_g$, which is called the *group velocity* (while $v_p(k) = \omega(k)/k$ is the phase velocity). If $v_g > 0$ i.e. if the function $\omega(k)$ is increasing in $k_0$, the packet translates in the positive direction of the $x$-axis (progressive propagation, as in Fig. 2). Vice versa, if $\omega(k)$ is decreasing in $k_0$ (regressive propagation).
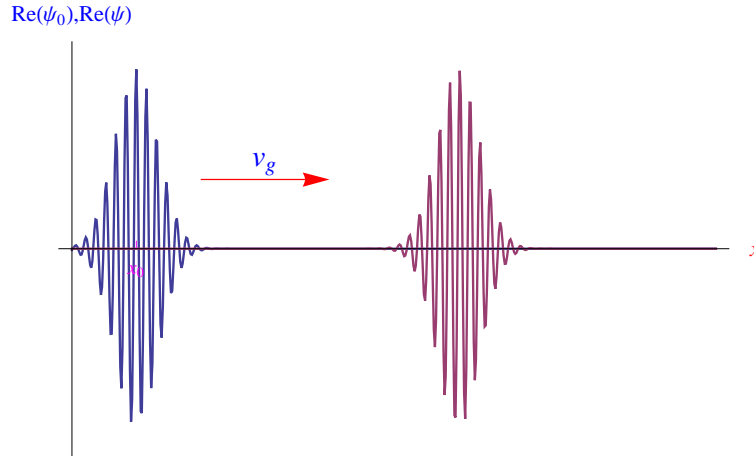


Figure 2: Progressive propagation of a wave packet.

Furthermore:

$$v_g = 0 \implies \psi(x,t) = e^{i\Omega_0 t} \psi_0(x)$$

which describes a standing wave. It is common to come across the following statement: «energy transport occurs at the group velocity». In reality, in the quantum mechanical state described by (3) the energy is not defined, since the initial state is a superposition of energy eigenstates. And such will be the state at all times:

$$\psi(x,t) = \int_{\sigma_c(\hat{H})} c^{(0)}(E) u_E(x) e^{-\frac{i}{\hbar}Et} dE \tag{15}$$

To define the energy we must perform a measurement operation, determining the "reduction" of the wave packet into one of the component monochromatic waves. If at $t = t_1$ we perform the measurement:

$$\psi(x,t) = \int_{\sigma_c(\hat{H})} c^{(0)}(E) u_E(x) e^{-\frac{i}{\hbar}Et} dE \xrightarrow[\text{mis}]{} u_E(x) e^{-\frac{i}{\hbar}E_1 t_1}$$

That is, the packet is reduced to the standing wave $u_E(x) e^{-\frac{i}{\hbar} E_1 t_1}$ and the result of the measurement is the eigenvalue $E_1$. We can still determine the expectation value of the energy on the state (15):

$$\langle E \rangle_{\psi(t)} = \left\langle \psi(t) \left| \hat{H} \right| \psi(t) \right\rangle = \left\langle \psi_0 \left| e^{\frac{i}{\hbar} t \hat{H}} \hat{H} e^{\frac{i}{\hbar} t \hat{H}} \right| \psi_0 \right\rangle = \left\langle \psi_0 \left| \hat{H} \right| \psi_0 \right\rangle = \langle E \rangle_{\psi_0}, \quad \forall t \geq 0 \quad (16)$$

This result is not surprising because the expectation value of any observable that commutes with the Hamiltonian does not depend on time. Regarding the group velocity:

$$v_g = \frac{1}{\hbar} \left. \frac{dE(k)}{dk} \right|_{k=k_0} \quad (17)$$

so the greater the rate of variation of $E$ as a function of $k$, the greater will be $|v_g|$. Of course, E is the energy of the single component of the wave packet and not the transported energy. All this in linear approximation. But if the medium is highly dispersive, i.e. if $\omega(k)$ varies rapidly even in a sufficiently small neighborhood of $k_0$, we cannot neglect the terms of order higher than the first in the series expansion of $\omega(k)$. In this case the packet does not translate rigidly and uniformly, and it is not possible to define a group velocity. This propagation process is known as *scattering*. This suggestive definition arises from the fact that the component waves have velocities so different from each other that they appear to propagate independently.

# 3   Dissipative effects

In this section we are no longer referring to a quantum system of the free particle type or subject to a periodic potential. The results we have reached in the previous section apply to other types of waves, such as packets of electromagnetic waves propagating in a dispersive medium. Here it makes physical sense to introduce dissipative effects, which are usually schematized by an exponential damping controlled by a coefficient $\beta > 0$:

$$\psi(x,t) = e^{-\beta x} \int_{-\infty}^{+\infty} A(k) e^{i(kx-\omega(k)t)} dk \quad (18)$$

However, in this schematization the individual monochromatic components undergo the same damping; it is more realistic, instead, to consider a damping that depends on $k$ and therefore on $\omega$ through the dispersion law $\omega(k)$. In this framework, dispersion and dissipation are intertwined processes. Furthermore, since in the theory of wave propagation, the phase plays a key role, we have to consider a complex attenuation factor:

$$\tau(k) = |\tau(k)| e^{i\phi(k)}, \qquad |\tau(k)| < 1 \quad (19)$$

So

$$\psi(x,t) = \int_{-\infty}^{+\infty} |\tau(k)| A(k) e^{i(kx-\omega(k)t+\phi(k))} dk \quad (20)$$

Recall that $|A(k)|$ is a Gaussian centered at $k_0$ and sufficiently peaked. If $\omega(k)$ and $\phi(k)$ do not vary rapidly in a suitable neighborhood of $k$, we can develop these functions there in a Taylor series truncated to first order:

$$\omega(k) \simeq \omega_0 + v_g(k-k_0), \quad \omega_0 \overset{def}{=} \omega(k_0), \quad v_g \overset{def}{=} \left. \frac{d\omega(k)}{dk} \right|_{k=k_0} \quad (21)$$

$$\phi(k) \simeq \phi_0 + \Lambda_0(k-k_0), \quad \phi_0 \overset{def}{=} \phi(k_0), \quad \Lambda_0 \overset{def}{=} \left. \frac{d\phi(k)}{dk} \right|_{k=k_0}$$

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Note that $\Lambda_0$ has the dimensions of a length. In this order of approximation

$$\psi\left(x,t\right) = \exp\left[i\left(-\omega_0 t + k_0 v_g t - \Lambda_0 k_0 + \phi_0\right)\right] \int_{-\infty}^{+\infty} \left|\tau\left(k\right)\right| A\left(k\right) \exp\left[ik\left(x - v_g t + \Lambda_0\right)\right] dk$$

Rearranging the various terms:

$$\psi\left(x,t\right) = e^{i\left(\Omega_0 t + \phi_0 - \Lambda_0 k_0\right)} \int_{-\infty}^{+\infty} B\left(k\right) e^{ik\left(x - v_g\left(t - T_0\right)\right)} dk$$

where $B\left(k\right) = \left|\tau\left(k\right)\right| A\left(k\right)$, while

$$T_0 = \frac{\Lambda_0}{v_g} \tag{22}$$

which physically represents the time taken by the packet to travel a length $\Lambda_0$. From (22)

$$T_0 = \frac{\left.\frac{d\phi(k)}{dk}\right|_{k=k_0}}{\left.\frac{d\omega(k)}{dk}\right|_{k=k_0}} = \left.\frac{d\phi}{d\omega}\right|_{\omega=\omega_0} \tag{23}$$

In other words, the linear approximation returns three characteristic quantities: 1) the group velocity $v_g$ which takes into account the dispersive effects; 2) the characteristic length $\Lambda_0$ which takes into account the dissipative effects; 3) the characteristic time $T_0$ which arises from a mix of the dispersive and dissipative effects. The time $T_0$ is called *group delay*. This expression derives from the fact that it expresses a phase delay or advance. Incidentally from (23), we have a delay $T_0 > 0$ if the function $\phi\left(\omega\right)$ is increasing in $\omega_0$. Instead, we have a group advance $T_0 < 0$, if $\phi\left(\omega\right)$ is decreasing in $\omega_0$.

# References

[1] Stratton J.A., *Electromagnetic Theory.*

[2] Experimental evidence that a photon can spend a negative amount of time in an atom cloud .

[3] Colozzo M., Motion of a Wave Packet.

[4] Jackson J.D., *Classical Electrodynamics.* Wiley.