Motion of a wave packet

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Abstract

We study the propagation of a wave packet in a dispersive medium, showing the existence of a cut-off in correspondence with the relative maximum/minimum points and the horizontal tangent inflections of the dispersion curve.

1 The D'Alembert equation and the Schrödinger equation

The D'Alembert wave equation and the Schrödinger wave equation share a special class of solutions, known as monochromatic plane waves.

Without loss of generality, we consider the one-dimensional case. The D'Alembert equation is written:

$$\frac{\partial^2 \psi}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 \psi}{\partial t^2} = 0 \tag{1}$$

Here c is a constant that is identified with the propagation speed of the wave described by the solution $\psi(x,t)$. The Schrödinger equation for a particle of mass m subjected to a potential energy field $V(x)$, is

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi(x,t) = i\hbar\frac{\partial \psi}{\partial t} \tag{2}$$

While in (1) is $\psi : \mathbb{R}^2 \to \mathbb{R}$, in (2) is $\psi : \mathbb{R}^2 \to \mathbb{C}$. Another important difference between the aforementioned equations is that the first is a PDE of the second order in the time derivative, while the second is a PDE of the first order with respect to the same derivative.

For (2) we are interested in the case $V(x) = 0$ which corresponds to the motion of a free particle:

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2mi}{\hbar}\frac{\partial \psi}{\partial t} = 0 \tag{3}$$

Solutions of the monochromatic plane wave type are written (in complex notation):

$$\psi(x,t) = Ae^{i(kx-\omega t)} \tag{4}$$

where $A > 0$ is the amplitude, while $k, \omega \in \mathbb{R}$ sare the *wave number* and the *angular frequency* (or pulsation) respectively. Note that ω and k are not independent, but linked by a relationship that depends on the PDE considered. Precisely by imposing that (4) is a solution of (1), we find:

$$\omega(k) = ck \tag{5}$$

By imposing that (3) is a solution of (1)

$$\omega(k) = \frac{\hbar k^2}{2m} \tag{6}$$

From classical electrodynamics it is known that the solutions of (1) represent electromagnetic waves in vacuum. From wave mechanics we know that the solutions of (2) describe the so-called matter waves or De Broglie waves (also called De Broglie - Schrödinger systems). In summary:

$$\omega(k) = \begin{cases} ck, & \text{onde elettromagnetiche nel vuoto} \\ \frac{\hbar k^2}{2m}, & \text{onde di De Broglie} \end{cases} \tag{7}$$

In other words, the function $\omega(k)$ is linear for electromagnetic waves in vacuum, and is quadratic for matter waves (even in the absence of forces). In the paradigm of old quantum theory, (5) has a notable physical interpretation. In fact, the momentum of the free particle is linked to the wave number of the De Broglie wave by $p = \hbar k$, while from the Planck-Einstein relation

$$E = \hbar\omega = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m}$$

that is, the energy of the free particle in classical motion.

2 The motion of wave packets. The law of dispersion

Let's rewrite (4)

$$\psi(x,t) = Ae^{i(kx-\omega(k)t)} \tag{8}$$

where $\omega(k)$ is given by (6). Remember that the number of waves is related to the wavelength λ by

$$k = \frac{2\pi}{\lambda} \tag{9}$$

so k is the number of complete oscillations in a length equal to 2π. Nella (9) is $k > 0$, but we can consider values < 0 which describe regressive waves i.e. propagating along the negative direction of the x axis. In this case the first member of (9) must be replaced with the absolute value given that $\lambda > 0$. The pulsation is instead linked to the frequency ν from $\omega = 2\pi\nu$.

That said, a monochromatic plane wave is a useful idealization since any light source exhibits inevitable frequency dispersion. In the case of radio waves, for example, no matter how tuned a transmitter/receiver may be, there will still be frequency dispersion. Simply put, the actual signal is a superposition of monochromatic waves. Assuming a linear superposition, the resulting wave is described by a function $\psi(x,t)$ which solves the D'Alembert equation, thanks to the linearity of the latter. We have thus constructed a wave packet. For the above, it is preferable to label the individual waves of the packet with the wave number k, rather than with the frequency. Then we write the wave function of the individual monochromatic components:

$$f(x,t;k) = A(k)\, e^{i(kx-\omega(k)t)} \tag{10}$$

where is the ; warns us that k is a parametric variable. The function $A(k)$ i.e. the amplitude of a single component. By virtue of the linearity of (1)-(3), the function

$$\psi(x,t) = \int_{-\infty}^{+\infty} A(k)\, e^{i(kx-\omega(k)t)} dk \tag{11}$$

it is still a solution of the aforementioned equations, with $\omega(k)$ given by (7). In cases of physical interest, $A(k)$ is extremely peaked around an assigned value k_0. It follows that denoting the width of the distribution with $2\Delta k$, we have

$$\psi(x,t) \simeq \int_{k_0-\Delta k}^{k_0-\Delta k} A(k)\, e^{i(kx-\omega(k)t)} dk \tag{12}$$

which has a simple physical interpretation: the dominant contribution to the resulting wave comes from the monochromatic components of wave number $k \in [k_0 - \Delta k, k_0 + \Delta k]$.

Assuming $\omega(k)$ analytical function:

$$\omega(k) = \sum_{n=0}^{+\infty} \frac{1}{n!} \left. \frac{d^n \omega(k)}{dk^n} \right|_{k=k_0} (k - k_0)^n \tag{13}$$

If $\omega(k)$ varies slowly around k_0, we can truncate the Taylor expansion (13) to first order:

$$\omega(k) \simeq \omega_0 + \left. \frac{d\omega(k)}{dk} \right|_{k=k_0} (k - k_0)^n, \quad (\omega_0 = \omega(k_0)) \tag{14}$$

Substituting in (11):

$$\psi(x,t) \simeq e^{i\left(k_0 \frac{d\omega(k)}{dk}\big|_{k=k_0} - \omega_0\right)t} \int_{k_0-\Delta k}^{k_0-\Delta k} A(k)\, e^{ik\left(x - \frac{d\omega(k)}{dk}\big|_{k=k_0} t\right)} dk \tag{15}$$

If $x' = x - \left. \frac{d\omega(k)}{dk} \right|_{k=k_0} t$

$$\int_{k_0-\Delta k}^{k_0-\Delta k} A(k)\, e^{ikx'} dk = \psi(x', 0) \equiv \psi(x - v_g t)$$

having defined the quantity (with the dimensions of a velocity):

$$v_g \stackrel{def}{=} \left. \frac{d\omega(k)}{dk} \right|_{k=k_0} \tag{16}$$

so

$$\psi(x,t) \simeq e^{i\left(k_0 \frac{d\omega(k)}{dk}\big|_{k=k_0} - \omega_0\right)t} \psi(x - v_g t)$$

where the exponential is an inessential phase factor. Definitely:

$$\psi(x,t) \simeq \psi(x - v_g t) \tag{17}$$

We conclude that in linear approximation (14) the packet profile translates rigidly and uniformly with speed (16) which we call the *group velocity*. Note that (17) is exactly verified if $\omega(k)$ è lineare is linear (and not a first-order truncated Taylor expansion), as in the case of a propagating electromagnetic packet in the void. For De Broglie waves, however, the $\omega(k)$ is quadratic and the translation of the packet is no longer rigid, in the sense that its profile deforms. Precisely, it tends to expand resulting in the so-called *scattering* of the packet. In Fig. 1 illustrates the propagation of a Gaussian De Broglie wave packet (i.e. for which $A(k)$ is a Gaussian centered in an assigned k_0).

Result:

$$v_g = \frac{d^2\omega(k)}{dk} = \frac{\hbar k}{m} = \frac{p}{m}$$

that is, the group velocity of the De Broglie packet is identified with the classical velocity of the particle.

In general, the function $\omega(k)$ defines the *dispersion law* of the medium in which the packet propagates. We have seen that in the case of a single monochromatic wave solving

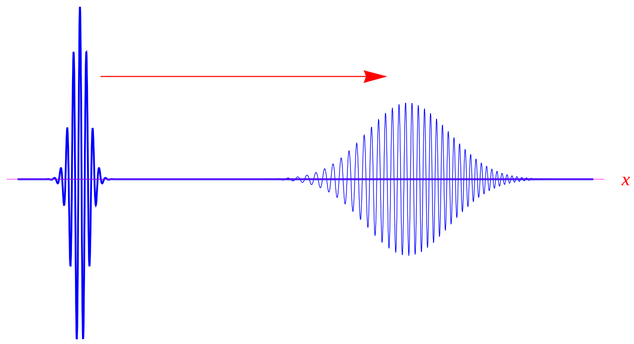

Figure 1: Gaussian wave packet in a dispersive medium with quadratic $\omega(k)$.

the D'Alembert equation is $c = \omega/k$. If such a wave composes a packet, then the previous quantity can be redefined as:

$$v_f = \frac{\omega(k)}{k} \tag{18}$$

and is the *phase velocity* of the packet. For a packet of electromagnetic waves propagating in a vacuum, the two speeds coincide: $v_g = v_f$. For a De Broglie package:

$$v_f = \frac{\hbar k}{2m}, \quad v_g = \frac{\hbar k}{m} \tag{19}$$

That is, the group velocity is greater than the phase velocity. It is important to highlight that the transport of energy occurs at the group speed, so this is the physically significant quantity.

3 Standing waves

In (11) is $\omega = \omega(k)$. Otherwise, if $\omega(k) \equiv \omega_0$:

$$\psi(x,t) = e^{-i\omega_0 t} \underbrace{\int_{-\infty}^{+\infty} A(k) e^{ikx} dk}_{=\phi(x)} \tag{20}$$

so the wave function is factorized into a spatial part $\phi(x)$ and into a sinusoidal oscillation of frequency ω_0. As is known from the theory of wave propagation, the (20) describes a standing wave. In this case, the group velocity is identically zero.

4 A differential equation for phase velocity

We prove an interesting theorem, expressing the various quantities as a function of the wavelength.

Theorem 1 *For a given group velocity $v_g(\lambda)$ of a wave packet, the phase velocity is an integral of the differential equation:*

$$\lambda \frac{dv_f}{d\lambda} - v_f = v_g \tag{21}$$

Proof. From $\lambda = \frac{2\pi}{k}$ we have the composite function $\omega = \omega(\lambda(k))$, so

$$v_g = \frac{d\omega}{dk} = \frac{d\omega}{d\lambda}\frac{d\lambda}{dk} = -\lambda^2 \frac{d\omega}{d\lambda}$$

But $\omega = 2\pi\nu$

$$v_g(\lambda) = -\lambda^2 \frac{d\nu}{d\lambda} \tag{22}$$

Phase velocity

$$v_f = \frac{\omega(k)}{k} = \lambda\nu(\lambda) \tag{23}$$

It follows

$$\frac{dv_f}{d\lambda} = \nu(\lambda) + \lambda\frac{d\nu}{d\lambda} \Longrightarrow \frac{d\nu}{d\lambda} = \frac{1}{\lambda}\frac{dv_f}{d\lambda} - \frac{1}{\lambda}\nu(\lambda)$$

which replaced in (22):

$$v_g(\lambda) = -\lambda\frac{dv_f}{d\lambda} + \underbrace{\lambda\nu(\lambda)}_{=v_f}$$

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(21) is a linear and non-homogeneous first-order differential equation[1]. Note that $\lambda = 0$ is a singular point. The general integral is

$$v_f(\lambda) = \frac{C}{\lambda} + \int \frac{v_g(\lambda)}{\lambda} d\lambda \tag{24}$$

C is a constant of integration. From (24) it follows that $v_f(\lambda)$ cannot be identically zero if is not $v_g(\lambda)$. But the opposite is not true:

$$v_g(\lambda) \equiv 0 \not\Rightarrow v_f(\lambda) \equiv 0$$

Infact from (24):

$$v_g(\lambda) \equiv 0 \Longrightarrow v_f(\lambda) = \frac{C}{\lambda}$$

remembering that as seen in § 3 for $v_g(\lambda) \equiv 0$ have a standing wave.

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Alternatively, the (21) can be interpreted as a relation linking the group velocity to the phase velocity. Incidentally

$$\frac{dv_f}{d\lambda} = 0 \Longrightarrow v_g = v_f$$

confirming the conclusions obtained previously. Note that for De Broglie waves it is $\frac{dv_f}{d\lambda} < 0$; to be convinced of this, simply apply the rule of derivation of composite functions to the function $v_f(k(\lambda))$.

[1]Linearity is a consequence of the linearity of the wave equation considered.

5 Cut-off of a wave packet. Bloch package

Another important class of solutions is given by amplitude-modulated plane waves. Precisely, if the potential energy field in which the particle moves is a periodic function $V(x)$ of period a, the energy eigenfunctions are plane waves modulated in amplitude and the modulation envelope is in turn a function periodic of period a [1]. It follows that if the particle is initially prepared in an energy eigenstate, the wavefunction at all times is

$$\phi_k(x,t) = \varphi_k(x)\, e^{i(kx-\omega(k)t)} \tag{25}$$

Here k is a "good quantum number" and has the dimensions of a pulse. Obviously it is not the momentum of the particle since this is not a constant of motion. Please note that $\omega(k)$ does not follow a quadratic law as in the case of De Broglie waves for a free particle. It is easy to persuade oneself that $\omega(k)$ is periodic with period $\frac{2\pi}{a}$.

In the general case, the particle is prepared in a *Bloch wave* superposition (25), i.e. its wavefunction at all times is a *Bloch package*

$$\psi(x,t) = \int_{k_0-\Delta k}^{k_0-\Delta k} A(k)\, \varphi_k(x)\, e^{i(kx-\omega(k)t)} dk \tag{26}$$

As stated, the function $\omega(k)$ which expresses the dispersion law, is a periodic function of period $\frac{2\pi}{a}$, and is non-negative and limited:

$$0 < \omega(k) \leq \Omega$$

We expect a symmetry in the propagation, hence the parity $(+1)$: $\omega(-k) \equiv \omega(k)$. Periodicity implies the existence of a countable infinity of critical points i.e. points where the first derivative $\omega'(k) = \frac{d\omega(k)}{dk}$. Remember that these points are points of relative maximum/minimum or points of inflection at a horizontal tangent. In the fundamental interval $\left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$ let k_* a critical point. It follows

$$\omega'(k_*) = 0 \Longrightarrow \omega'\left(k_* + \frac{2\pi n}{a}\right) = 0, \quad \forall n \in Z$$

So

$$v_g\left(k_* + \frac{2\pi n}{a}\right) = 0, \quad \forall n \in Z \tag{27}$$

Definition 2 *The values of the number of waves k for which the group velocity vanishes are called wave packet cut-off.*

As seen in § 3, it follows the existence of a countable infinity of cut-offs of a Bloch package.

References

[1] Colozzo.M., A Very Simple Proof of the Bloch's Theorem.

[2] https://www.amazon.com/Classical-Electrodynamics-Third-David-Jackson/dp/047130932X.