Group velocity in a crystal lattice*

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Abstract

[In this note we point out the existence in real media—crystal lattices—of a range of frequencies with negative group velocity, i. e., group velocity which is directed oppositely to the phase velocity.]

The usual ideas of phase and group velocity are applied to waves in continuous homogeneous media. The situation with which we almost always deal is one where the group velocity $d\omega/dk$, being in the presence of dispersion different in value from the phase velocity ω/k (ω is the frequency, k is the wave number), nonetheless has the same direction. In these cases it is said that the group velocity is positive.

We should perhaps emphasize that the nature of such phenomena depends essentially on the sign of the group velocity, because the group velocity is ordinarily not mentioned in connection with the analysis.

I have in mind, for example, the reflection and refraction of a plane wave at the interface between two nonabsorbing media.

In the derivation of the corresponding relations—the direction of the refracted ray, the values of the amplitudes of the reflected and refracted waves—a large part is played by an unstated assumption: that the direction of the phase velocity of the refracted wave forms an *acute* angle with the normal to the interface (directed into the "second" medium).

But in accordance with the meaning of the physical problem, this assumption must be imposed on the group velocity (to the velocity of energy propagation). A valid result is obtained only when, as indicated above, the actual case deals with positive group velocity.

{For negative group velocity, the requirement of outward flow of energy from the interface is tantamount to the requirement of the motion of the phase toward this interface. In this case, the refracted ray is oriented not in the usual way, but along a direction flipped relative to the normal in comparison to the usual direction. Certainly, it is also numerically different from the usual one. Thus,

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the phenomena of reflection and refraction depend essentially on the sign of the group velocity.}[1]

As is known, Lamb worked out several cases of *fictitious* one-dimensional media with negative group velocities.[2]

Lamb himself evidently did not regard the examples he provided as having physical application. {He saw their significance in this way: "…the preceding discussion may serve to emphasize the point that ideas of wave-propagation acquired in the study of air-waves (for example) need to be used with some caution when we are dealing with a dispersive medium".}

In the present note, I want to direct attention to the fact that there exist real media for which the phase and group velocities have in fact opposite directions within certain frequency ranges. I have in mind wave propagation in crystal lattices. It is important to note, however, that when we speak of waves—for example, plane harmonic waves—in such lattices, we are not speaking yet of the necessity of accounting for the discrete structure of the medium; we have in mind a certain extension of the ordinary notion of a "wave".

Specifically, by a plane wave is to be understood a *complex* of plane waves of a single frequency, a single direction and wave number, but with various amplitudes. Each of the n waves of the complex (where n is the number of basis points of the lattice) determines the displacement of homologous points of the lattice as functions of the spatial coordinates and time.

It is known that each of the given values of the wave number k corresponds to n different values of the frequency $\omega_i^{(k)}$ $(i = 1, 2, \ldots, n)$.

For many applications, as Born indicates in this connection, the important waves are those whose wavelengths are large compared to the lattice constant. I would remark that it is this very case which is important to us, for example, in problems of molecular light scattering in crystals.

Born also showed the following: if we denote by $\omega_i^{(0)}$ the frequencies corresponding to the value $k = 0$, then near each of these values (which, generally speaking, separate real values of the wavenumber from imaginary ones), the frequency can be expanded into a power series in k. That value of $\omega_i^{(0)}$ which tends to zero simultaneously with k corresponds to the "acoustic spectrum." The amplitudes of the separated wave complex here become equal to each other when $k = 0$.

These very types of oscillations are approximated by considering the crystal as a continuous medium. In the acoustic region of the spectrum, the group velocity is positive.

We are interested in the "optical" region of the spectrum, where

$$(\omega_i^{(k)})^2 = (\omega_i^{(0)})^2 + a_i^{(1)} k + a_i^{(2)} k^2 + \ldots,$$

in which $\omega_i^{(0)} \neq 0$. In the nondegenerate case when $a_i^{(1)} = 0$, it is likewise easy

[1] Curly brackets { } indicate insertions made from the rough draft.

[2] [Translator's note: H. Lamb, "On group-velocity," *Proc. London Math. Soc.*, ser. 2, vol. 1, pp. 473-479, 1904.]

to show that $a_i^{(2)}$ can be either positive or negative. In the latter case we will have negative group velocity.

The relations herein are easy to follow in the one-dimensional case of longitudinal oscillations of a chain, consisting of an alternating sequence of equidistant masses m_1, m_2, …, m_n, in which each is connected with its neighbors by a quasi-elastic spring with a constant spring coefficient f. Here one can show the following.

If the frequencies $\omega_i^{(0)}$ are arranged in increasing order, beginning with $\omega_1^{(0)} = 0$, then, firstly, of course, all $a_i^{(1)} = 0$, and $a_i^{(2)}$ is positive for odd indices i and negative for even i, i. e., the regions of the spectrum in which the group velocity is positive alternate with regions in which it is negative.

I believe that analogous results will prove to be true for rather general cases of three-dimensional lattices.

Perhaps it is best to carry out as an illustration of the assertions concerning this chain a very simple example, namely the case of two different alternating masses m_1 and m_2, located at distances d from each other. Here

$$\omega_1^2 = \frac{2k^2 d^2 f}{m_1 + m_2} + \ldots,$$

$$\omega_2^2 = 2f\frac{m_1 + m_2}{m_1 m_2} - \frac{2d^2 f}{m_1 + m_2}k^2.$$

Thus, in the optical spectrum the group velocity is

$$\frac{d\omega}{dk} = -\frac{2kd^2 f}{(m_1 + m_2)\omega_2^{(0)}}.$$

From this example it is easy to to convince oneself that the energy in the chain is propagated at the group velocity. Here, the energy propagation velocity W *by definition* (due to Lord Rayleigh) has the following value:

$$W = \bar{P}/\bar{E}$$

where $\bar{P}$ is the time-average value of the "Poynting vector", while $\bar{E}$ is the average value of the energy per unit length.

If by ξ_l (where l is even) we denote the displacements of the particles of mass m_2, by ξ_l with odd index the displacements of the masses m_1 ($l = \ldots, -3, -2, -1, 0, 1, 2, \ldots$), and by b and a the amplitudes of the corresponding waves, then it is easy to see that the one-dimensional Poynting vector has the form

$$P = f(\xi_{m-1} - \xi_m)\dot{\xi}_m.$$

A simple calculation gives

$$\bar{P} = \frac{\omega_2^{(0)}}{2} fab \sin kd$$

Thus, $\bar{P}$ is indeed invariant for all particles of the lattice.

We further have

$$\bar{E} = \frac{(m_1 a^2 + m_2 b^2)(\omega_2^{(0)})^2}{4d} \qquad \text{and} \qquad \frac{a}{b} = -\frac{m_2}{m_1}.$$

Hence,

$$W = \frac{\bar{P}}{\bar{E}} = -\frac{2}{\omega_2^{(0)}} \frac{fkd^2}{(m_1 + m_2)}, \qquad \text{i. e.} \qquad W = \frac{d\omega}{dk}.$$

It only remains perhaps to make the following remarks. In the degenerate case $m_1 = m_2$ the preceding considerations remain in force. But here there exists, also in contrast to the general case, one harmonic wave (with wavelength on the order of d), which covers both the even and odd mass points. The velocity of phase propagation of this wave has the same direction as the group velocity and not the opposite, which certainly in no way contradicts the preceding results. In conclusion I want to note also the following.

A crystal lattice is a limiting case of a continuous medium with periodically varying parameters (density, permittivity, etc.).

Considerations related to wave propagation in lattices that were indicated above can likewise be extended to such media; this will certainly cover more than just the case of elastic waves. Specifically here too, particularly for "long waves", it is suitable to speak of group velocity, which also in this case becomes negative in certain ranges. Without going into a detailed consideration of these questions, I will remark only by way of example on the propagation of waves in the x-direction in a medium whose properties depend only on x. The problem of the propagation of oscillations in such a medium is known to lead to Hill's equation. There exist two "waves":

$$f_1(x)e^{i(kx+\omega t)} \qquad \text{and} \qquad f_2(x)e^{i(-kx+\omega t)}$$

where f_1 and f_2 are functions periodic with the period of the medium. The number of discrete values of frequency corresponding to $k = 0$ is infinite here (the boundaries between stable and unstable regions). If, for example, the material property of the medium (the dielectric constant ϵ, say) has the form

$$\epsilon = \epsilon_0 + \epsilon_1 \cos \mu x$$

then it is easy to show that the spectral regions with positive and negative velocities alternate with each other.