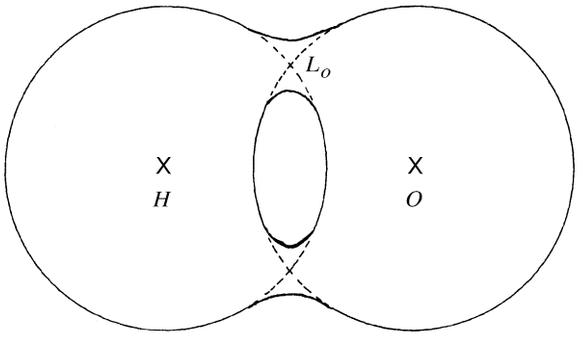

Fig. 5.1.2.3. Intersection of the dispersion surface with the plane of incidence. The dispersion surface is a connecting surface between the two spheres centred at reciprocal-lattice points O and H and with radius nk. L_o is the Lorentz point.

propagate in the crystal with a given frequency. This locus is called the *dispersion surface*. It is a constant-energy surface and is the equivalent of the index surface in optics. It is the X-ray analogue of the constant-energy surfaces known as Fermi surfaces in the electron band theory of solids.

In the two-beam case, the dispersion surface is a surface of revolution around the diffraction vector **OH**. It is made from two spheres and a connecting surface between them. The two spheres are centred at O and H and have the same radius, nk. Fig. 5.1.2.3 shows the intersection of the dispersion surface with a plane passing through **OH**. When the tie point lies on one of the two spheres, far from their intersection, only one wavefield propagates inside the crystal. When it lies on the connecting surface, two waves are excited simultaneously. The equation of this surface is obtained by equating to zero the determinant of system (5.1.2.20):

$$X_o X_h = k^2 C^2 \chi_h \chi_{\bar{h}}/4. \qquad (5.1.2.22)$$

Equations (5.1.2.21) show that, in the zero-absorption case, X_o and X_h are to be interpreted as the distances of the tie point P from the spheres centred at O and H, respectively. From (5.1.2.20) it can be seen that they are of the order of the vacuum wavenumber times the Fourier coefficient of the dielectric susceptibility, that is five or six orders of magnitude smaller than k. The two spheres can therefore be replaced by their tangential planes. Equation (5.1.2.22) shows that the product of the distances of the tie point from these planes is constant. The intersection of the dispersion surface with the plane passing through **OH** is therefore a hyperbola (Fig. 5.1.2.4) whose diameter [using (5.1.2.5) and (5.1.2.22)] is

$$\overline{A_{o2}A_{o1}} = |C|R\lambda(F_h F_{\bar{h}})^{1/2}/(\pi V \cos\theta). \qquad (5.1.2.23)$$

It can be noted that the larger the diameter of the dispersion surface, the larger the structure factor, that is, the stronger the interaction of the waves with the matter. When the polarization is parallel to the plane of incidence ($C = \cos 2\theta$), the interaction is weaker.

The asymptotes T_o and T_h to the hyperbola are tangents to the circles centred at O and H, respectively. Their intersection, L_o, is called the *Lorentz point* (Fig. 5.1.2.4).

A wavefield propagating in the crystal is characterized by a tie point P on the dispersion surface and two waves with wavevectors $\mathbf{K_o} = \mathbf{OP}$ and $\mathbf{K_h} = \mathbf{HP}$, respectively. The ratio, ξ, of their amplitudes D_h and D_o is given by means of (5.1.2.20):

$$\xi = \frac{D_h}{D_o} = \frac{2X_o}{kC\chi_{\bar{h}}} = \frac{-2\pi V X_o}{R\lambda C F_{\bar{h}}}. \qquad (5.1.2.24)$$

The hyperbola has two branches, 1 and 2, for each direction of polarization, that is, for $C = 1$ or $\cos 2\theta$ (Fig. 5.1.2.5). Branch 2 is

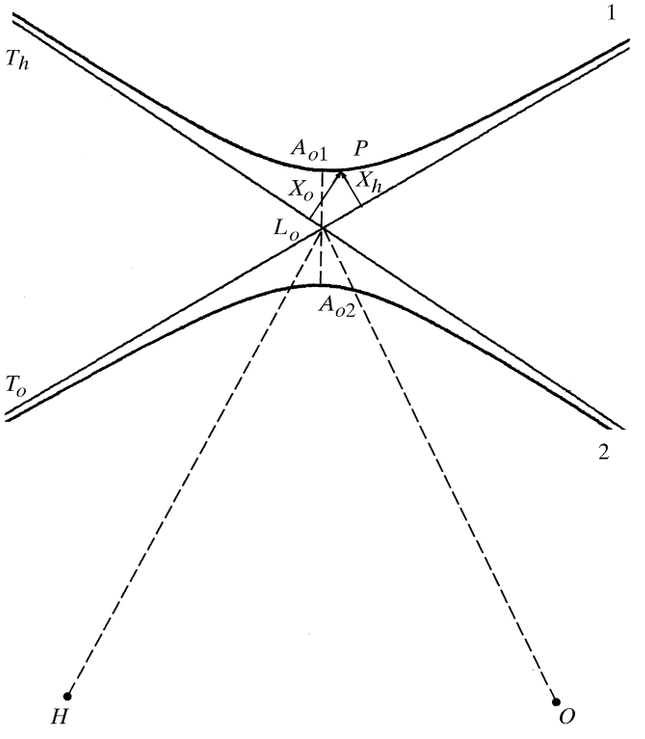

Fig. 5.1.2.4. Intersection of the dispersion surface with the plane of incidence shown in greater detail. The Lorentz point L_o is far away from the nodes O and H of the reciprocal lattice: $OL_o = HL_o = 1/\lambda$ is about 10^5 to 10^6 times larger than the diameter $A_{o1}A_{o2}$ of the dispersion surface.

the one situated on the same side of the asymptotes as the reciprocal-lattice points O and H. Given the orientation of the wavevectors, which has been chosen away from the reciprocal-lattice points (Fig. 5.1.2.1*b*), the coordinates of the tie point, X_o and X_h, are positive for branch 1 and negative for branch 2. The phase of ξ is therefore equal to $\pi + \varphi_h$ and to φ_h for the two branches, respectively, where φ_h is the phase of the structure factor [equation (5.1.2.6)]. This difference of π between the two branches has important consequences for the properties of the wavefields.

As mentioned above, owing to absorption, wavevectors are actually complex and so is the dispersion surface.

5.1.2.6. *Propagation direction*

The energy of all the waves in a given wavefield propagates in a common direction, which is obtained by calculating either the group velocity or the Poynting vector [see Section A5.1.1.4, equation (A5.1.1.8) of the Appendix]. It can be shown that, averaged over time and the unit cell, the Poynting vector of a wavefield is

$$\mathbf{S} = (c/\varepsilon_0)\exp(4\pi\mathbf{K_{oi}}\cdot\mathbf{r})\left[|D_o|^2\mathbf{s_o} + |D_h|^2\mathbf{s_h}\right], \qquad (5.1.2.25)$$

where $\mathbf{s_o}$ and $\mathbf{s_h}$ are unit vectors in the $\mathbf{K_o}$ and $\mathbf{K_h}$ directions, respectively, c is the velocity of light and ε_0 is the dielectric permittivity of a vacuum. This result was first shown by von Laue (1952) in the two-beam case and was generalized to the n-beam case by Kato (1958).

From (5.1.2.25) and equation (5.1.2.22) of the dispersion surface, it can be shown that the propagation direction of the wavefield lies along the normal to the dispersion surface at the tie point (Fig. 5.1.2.5). This result is also obtained by considering the group velocity of the wavefield (Ewald, 1958; Wagner, 1959). The angle α

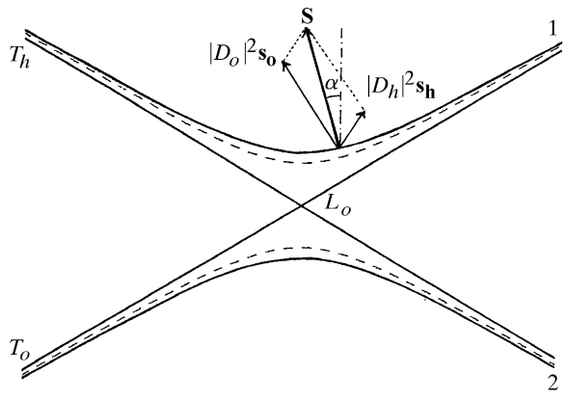

Fig. 5.1.2.5. Dispersion surface for the two states of polarization. Solid curve: polarization normal to the plane of incidence ($C = 1$); broken curve: polarization parallel to the plane of incidence ($C = \cos 2\theta$). The direction of propagation of the energy of the wavefields is along the Poynting vector, **S**, normal to the dispersion surface.

between the propagation direction and the lattice planes is given by

$$\tan\alpha = \left[(1 - |\xi|^2)/(1 + |\xi|^2)\right] \tan\theta. \qquad (5.1.2.26)$$

It should be noted that the propagation direction varies between $\mathbf{K_o}$ and $\mathbf{K_h}$ for both branches of the dispersion surface.

5.1.3. Solutions of plane-wave dynamical theory

5.1.3.1. *Departure from Bragg's law of the incident wave*

The wavefields excited in the crystal by the incident wave are determined by applying the boundary condition mentioned above for the continuity of the tangential component of the wavevectors (Section 5.1.2.3). Waves propagating in a vacuum have wavenumber $k = 1/\lambda$. Depending on whether they propagate in the incident or in the reflected direction, the common extremity, M, of their wavevectors

$$\mathbf{OM} = \mathbf{K_o^{(a)}} \text{ and } \mathbf{HM} = \mathbf{K_h^{(a)}}$$

lies on spheres of radius k and centred at O and H, respectively. The intersections of these spheres with the plane of incidence are two circles which can be approximated by their tangents T_o' and T_h' at their intersection point, L_a, or *Laue point* (Fig. 5.1.3.1).

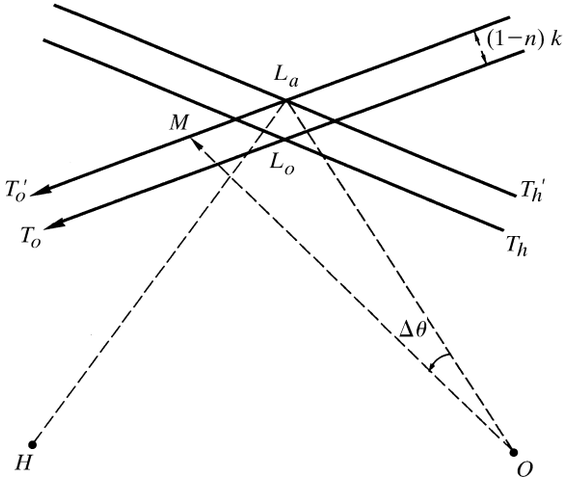

Fig. 5.1.3.1. Departure from Bragg's law of an incident wave.

Bragg's condition is exactly satisfied according to the geometrical theory of diffraction when M lies at L_a. The departure $\Delta\theta$ from Bragg's incidence of an incident wave is defined as the angle between the corresponding wavevectors **OM** and $\mathbf{OL}_a$. As $\Delta\theta$ is very small compared to the Bragg angle in the general case of X-rays or neutrons, one may write

$$\begin{aligned} \mathbf{K_o^{(a)}} &= \mathbf{OM} = \mathbf{OL}_a + \mathbf{L}_a\mathbf{M}, \\ \Delta\theta &= \overline{L_aM}/k. \end{aligned} \qquad (5.1.3.1)$$

The tangent T_o' is oriented in such a way that $\Delta\theta$ is negative when the angle of incidence is smaller than the Bragg angle.

5.1.3.2. *Transmission and reflection geometries*

The boundary condition for the continuity of the tangential component of the wavevectors is applied by drawing from M a line, **Mz**, parallel to the normal **n** to the crystal surface. The tie points of the wavefields excited in the crystal by the incident wave are at the intersections of this line with the dispersion surface. Two different situations may occur:

(*a*) *Transmission, or Laue case* (Fig. 5.1.3.2). The normal to the crystal surface drawn from M intersects *both* branches of the dispersion surface (Fig. 5.1.3.2*a*). The reflected wave is then directed towards the *inside* of the crystal (Fig. 5.1.3.2*b*). Let γ_o and γ_h be the cosines of the angles between the normal to the crystal surface, **n**, and the incident and reflected directions, respectively:

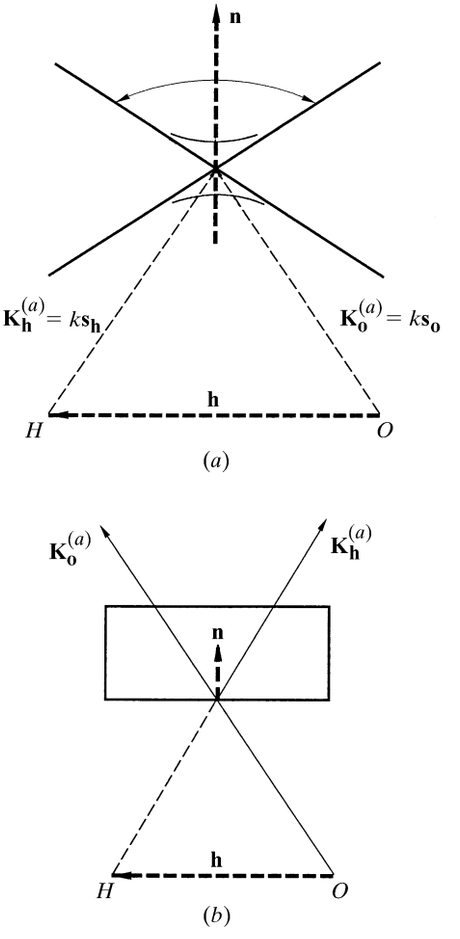

Fig. 5.1.3.2. Transmission, or Laue, geometry. (*a*) Reciprocal space; (*b*) direct space.

references