$$T_{mn} = \frac{k_B T}{8\pi^3} q_m \int\int \left(\mathbf{A}^{-1}\right)_{mn} \mathrm{d}S,$$

where q_m is the radius of the sphere that replaces the anisotropic region (Fig. 7.4.2.2) actually scanned in the experiment, and $\mathrm{d}S$ is a surface element of this sphere. q_m can be estimated by equating the volume of the sphere to the volume swept out in the scan.

If *both* approximations are employed, the correction factor is isotropic and reduces to

$$\alpha = \frac{H^2 k_B T q_m}{3\pi^2 \rho \mathbf{v}_L^2}, \qquad (7.4.2.14)$$

with $\mathbf{v}_L$ representing the mean velocity of the elastic waves, averaged over all directions of propagation and of polarization.

Experimental values of α have been measured for several crystals by γ-ray diffraction of Mössbauer radiation (Krec & Steiner, 1984). In general, there is good agreement between these values and those calculated by the numerical methods, which take into account anisotropy of the TDS. The correction factors calculated analytically from (7.4.2.14) are less satisfactory.

The principal effect of *not* correcting for TDS is to underestimate the values of the atomic displacement parameters. Writing $\exp\alpha \approx 1 + \alpha$, we see from (7.4.2.14) that the overall displacement factor is increased from B to $B + \Delta B$ when the correction is made. ΔB is given by

$$\Delta B = \frac{8 k_B T q_m}{3\pi^2 \rho \mathbf{v}_L^2}.$$

Typically, $\Delta B/B$ is 10–20%. Smaller errors occur in other parameters, but, for accurate studies of charge densities or bonding effects, a TDS correction of all integrated intensities is advisable (Helmholdt & Vos, 1977; Stevenson & Harada, 1983).

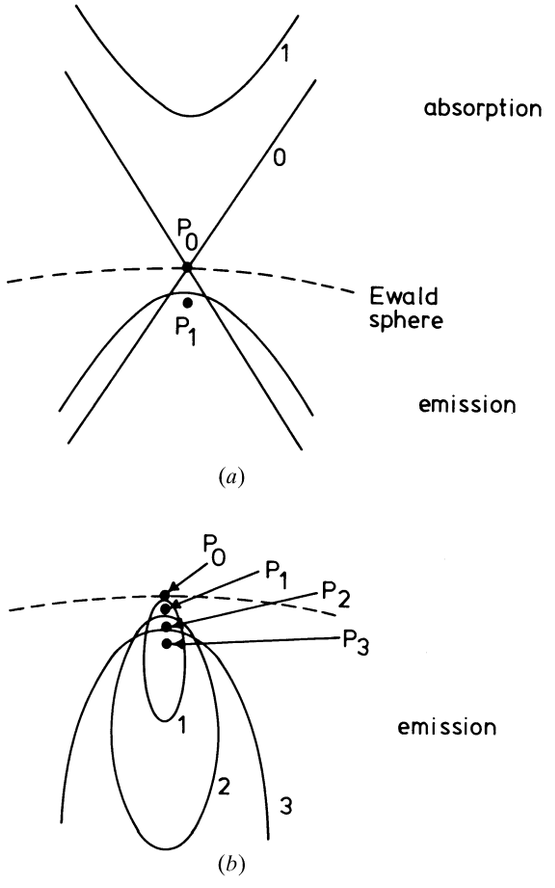

Fig. 7.4.2.3. Scattering surfaces for one-phonon scattering of neutrons: (*a*) for neutrons faster than sound ($\beta < 1$); (*b*) for neutrons slower than sound ($\beta > 1$). The scattering surface for X-rays is the Ewald sphere. P_0, P_1, *etc*. are different positions of the reciprocal-lattice point with respect to the Ewald sphere, and the scattering surfaces are numbered to correspond with the appropriate position of P.

7.4.2.3. *TDS correction factor for thermal neutrons (single crystals)*

The neutron treatment of the correction factor lies along similar lines to that for X-rays. The principal difference arises from the different topologies of the one-phonon 'scattering surfaces' for X-rays and neutrons. These surfaces represent the locus in reciprocal space of the end-points of the phonon wavevectors $\mathbf{q}$ (for fixed crystal orientation and fixed incident wavevector $\mathbf{k}_0$) when the wavevector $\mathbf{k}$ of the scattered radiation is allowed to vary. We shall not discuss the theory for pulsed neutrons, where the incident wavelength varies (see Popa & Willis, 1994).

The scattering surfaces are determined by the conservation laws for momentum transfer,

$$\mathbf{H} = \mathbf{k} - \mathbf{k}_0 = 2\pi\mathbf{h} + \mathbf{q},$$

and for energy transfer,

$$\hbar^2\left(k^2 - k_0^2\right)/2m_n = -\varepsilon\hbar\omega_j(\mathbf{q}), \qquad (7.4.2.15)$$

where m_n is the neutron mass and $\hbar\omega_j(\mathbf{q})$ is the phonon energy. ε is either $+1$ or -1, where $\varepsilon = +1$ corresponds to phonon emission (or phonon creation) in the crystal and a loss in energy of the neutrons after scattering, and $\varepsilon = -1$ corresponds to phonon absorption (or phonon annihilation) in the crystal and a gain in neutron energy. In the X-ray case, the phonon energy is negligible compared with the energy of the X-ray photon, so that (7.4.2.15) reduces to

$$k = k_0,$$

and the scattering surface is the Ewald sphere. For neutron scattering, $\hbar\omega_j(\mathbf{q})$ is comparable with the energy of a thermal neutron, and so the topology of the scattering surface is more complicated. For one-phonon scattering by long-wavelength acoustic modes with $q \ll k_0$, (7.4.2.15) reduces to

$$k = k_0 - \varepsilon\beta q,$$

where β ($= \mathbf{v}_L/\mathbf{v}_n$) is the ratio of the sound velocity in the crystal and the neutron velocity. If the Ewald sphere in the neighbourhood of a reciprocal-lattice point is replaced by its tangent plane, the scattering surface becomes a conic section with eccentricity $1/\beta$. For $\beta < 1$, the conic section is a hyperboloid of two sheets with the reciprocal-lattice point P at one focus. The phonon

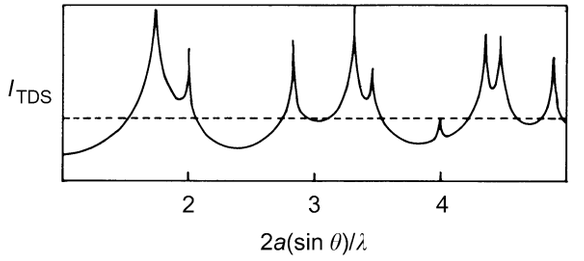

Fig. 7.4.2.4. One-phonon scattering calculated for polycrystalline nickel of lattice constant a (after Suortti, 1980).

references