Neglecting higher-order terms, summing up both sides of equation (2.1.2.30) over κ and multiplying by $\mathbf{u}_o$ yields

$$\begin{aligned} M\,\omega^2_{\mathbf{q}\to\mathbf{0},j}\,\mathbf{u}_o^2 &= \sum_{\kappa}\sum_{\kappa' l'}\sum_{\alpha\beta} u_o^\alpha\,\mathbf{V}_{\alpha\beta}(\kappa l,\kappa' l')\,u_o^\beta \\ &\quad + i\sum_\gamma q_\gamma \sum_{\kappa}\sum_{\kappa' l'}\sum_{\alpha\beta} u_o^\alpha\,V_{\alpha\beta}(\kappa l,\kappa' l')\,(r_{l'}^{o^\gamma} - r_l^{o^\gamma})\,u_o^\beta \\ &\quad - \tfrac{1}{2}\sum_\delta\sum_\gamma q_\gamma\,q_\delta \sum_{\kappa}\sum_{\kappa' l'}\sum_{\alpha\beta} u_o^\alpha\,V_{\alpha\beta}(\kappa l,\kappa' l') \\ &\quad \times (r_{l'}^{o^\gamma} - r_l^{o^\gamma})\,(r_{l'}^{o^\delta} - r_l^{o^\delta})\,u_o^\beta, \end{aligned} \tag{2.1.2.31}$$

M being the total mass of all atoms within the primitive cell ($M = \sum_{\kappa=1}^{N} m_\kappa$). The first term on the right-hand side is zero according to equation (2.1.2.29). The second term vanishes due to the symmetry property of the force-constant matrices, equation (2.1.2.23). Hence (2.1.2.31) is simplified to

$$\begin{aligned} M\left(\frac{\omega_{\mathbf{q}\to\mathbf{0},j}}{|\mathbf{q}|}\right)^2 &= -\tfrac{1}{2}\sum_\delta\sum_\gamma \frac{q_\gamma\,q_\delta}{\mathbf{q}^2}\sum_{\kappa}\sum_{\kappa' l'}\sum_{\alpha\beta} V_{\alpha\beta}(\kappa l,\kappa' l') \\ &\quad \times (r_{l'}^\gamma - r_l^\gamma)\,(r_{l'}^\delta - r_l^\delta)\,\frac{u_o^\alpha\,u_o^\beta}{\mathbf{u}_o^2}. \end{aligned} \tag{2.1.2.32}$$

The right-hand side no longer depends on the moduli of the wavevector and displacement but only on their orientation with respect to the crystal lattice. Consequently, acoustic dispersion curves always leave the Γ point as a straight line with a constant slope ($\omega/|\mathbf{q}|$).

The displacement pattern of these long-wavelength modes corresponds to a continuous deformation of a rigid body. Hence, acoustic phonons near the Γ point can be regarded as sound waves and the slope of the dispersion curve is given by the corresponding sound velocity,

$$v_s = \omega/|\mathbf{q}|. \tag{2.1.2.33}$$

Sound velocities, on the other hand, can be calculated from macroscopic elastic constants using the theory of macroscopic elasticity (*cf.* Chapter 1.3). Thus we are able to correlate macroscopic and microscopic dynamic properties of crystals. Using the generalized Hooke's law, the equation of motion for the dynamic deformation of a macroscopic body may be written as

$$\rho\frac{\partial^2 u_j(t)}{\partial t^2} = \sum_{k=1}^{3}\sum_{l=1}^{3}\sum_{m=1}^{3} c_{jklm}\frac{\partial^2 u_l}{\partial r^k\,\partial r^m}, \tag{2.1.2.34}$$

ρ being the macroscopic density, u_i the ith Cartesian component of the deformation and (c_{jklm}) the symmetric tensor of elastic stiffnesses, which is discussed in detail in Chapter 1.3. The solution of this differential equation using plane waves,

$$\mathbf{u} = \mathbf{u}_o\,\exp[i(\mathbf{q}\mathbf{r} - \omega t)], \tag{2.1.2.35}$$

leads to the following relation:

$$\rho\left(\frac{\omega}{|\mathbf{q}|}\right)^2 u_o^j = \sum_{k=1}^{3}\sum_{l=1}^{3}\sum_{m=1}^{3} c_{jklm}\frac{q_k\,q_m}{\mathbf{q}^2}u_o^l. \tag{2.1.2.36}$$

If we define the components of the *propagation tensor* by

$$\Gamma_{jl} = \sum_{k=1}^{3}\sum_{m=1}^{3} c_{jklm}\frac{q_k\,q_m}{\mathbf{q}^2}, \tag{2.1.2.37}$$

equation (2.1.2.36) may be written as the eigenvector equation

$$\rho\,v_s^2\,\mathbf{u}_o = \mathbf{\Gamma}\,\mathbf{u}_o. \tag{2.1.2.38}$$

For a given propagation direction as defined by the Cartesian components of $\mathbf{q}$, the eigenvectors of the corresponding propagation tensor yield the polarization of three mutually orthogonal deformation waves. Its eigenvalues are related to the respective sound velocities $v_s = \omega/|\mathbf{q}|$. If the tensor of elastic stiffnesses is known, the elements of $\mathbf{\Gamma}$ and, hence, the velocity of elastic (sound) waves can be calculated for arbitrary propagation directions (see Section 1.3.4). These data, in turn, allow the prediction of the slopes of acoustic phonon dispersion curves near $\mathbf{q} = \mathbf{0}$.

2.1.2.5. *Eigenvectors and normal coordinates*

The plane-wave solutions (2.1.2.10) of the equations of motion form a complete set of orthogonal functions if $\mathbf{q}$ is restricted to the first Brillouin zone. Hence, the actual displacement of an atom (κl) can be represented by a linear combination of the $\mathbf{u}_{\kappa l}^{\pm}(\mathbf{q}, j)$:

$$\mathbf{u}_{\kappa l} = \sum_{\mathbf{q}}\sum_{j}[A_{\mathbf{q},j}\,\mathbf{u}_{\kappa l}^{+}(\mathbf{q},j) + A'_{\mathbf{q},j}\,\mathbf{u}_{\kappa l}^{-}(\mathbf{q},j)]. \tag{2.1.2.39}$$

Since this displacement is an observable quantity, it must correspond to a real vector, not a complex one. Hence, the coefficients $A_{\mathbf{q},j}$ obey the relation

$$A'_{\mathbf{q},j} = A^*_{-\mathbf{q},j} \tag{2.1.2.40}$$

and equation (2.1.2.39) reduces to

$$\mathbf{u}_{\kappa l} = \frac{1}{\sqrt{N m_\kappa}}\sum_{\mathbf{q}}\sum_{j} Q_{\mathbf{q},j}\,\mathbf{e}_\kappa(\mathbf{q},j)\exp(i\mathbf{q}\mathbf{r}_l), \tag{2.1.2.41}$$

where

$$Q_{\mathbf{q},j} = A_{\mathbf{q},j}\,\exp(-i\omega_{\mathbf{q},j}t) + A^*_{-\mathbf{q},j}\,\exp(i\omega_{\mathbf{q},j}t) = Q^*_{-\mathbf{q},j}. \tag{2.1.2.42}$$

If the displacement vectors $\mathbf{u}_{\kappa l}$ are combined to form a $3N$-dimensional vector $\mathbf{u}_l$ in analogy to the formation of the eigenvector $\mathbf{e}(\mathbf{q}, j)$ from the individual polarization vectors $\mathbf{e}_\kappa(\mathbf{q}, j)$ [equation (2.1.2.18)] we obtain

$$\mathbf{u}_l = \frac{1}{\sqrt{N}}\sum_{\mathbf{q}}\sum_{j} Q_{\mathbf{q},j}\,\mathbf{M}\,\mathbf{e}(\mathbf{q},j)\,\exp(i\mathbf{q}\mathbf{r}_l). \tag{2.1.2.43}$$

Thus, the atomic displacement is a linear combination of the eigenvectors $\mathbf{e}(\mathbf{q}, j)$ of the dynamical matrix. The coefficients $Q_{\mathbf{q},j}$ are called *normal coordinates*. They reflect the relative weight and amplitude of a particular vibrational mode ($\mathbf{q}, j$) which is temperature-dependent and may be determined by statistical methods.

In terms of these normal coordinates, the Hamiltonian of the lattice (2.1.2.8) is reduced to a sum of independent harmonic oscillators. These are called *phonons* and may be regarded as quantum quasiparticles.

$$H = \frac{N_Z}{2N}\sum_{\mathbf{q}}\sum_{j}\left[\left|\frac{\mathrm{d}Q_{\mathbf{q},j}}{\mathrm{d}t}\right|^2 + \omega^2_{\mathbf{q},j}\left|Q_{\mathbf{q},j}\right|^2\right]. \tag{2.1.2.44}$$

(N_Z is the number of primitive cells within the crystal.)

2.1.2.6. *Amplitudes of lattice vibrations*

Lattice vibrations that are characterized by both the frequencies $\omega_{\mathbf{q},j}$ and the normal coordinates $Q_{\mathbf{q},j}$ are elementary excitations of the harmonic lattice. As long as anharmonic effects are neglected, there are no interactions between the individual phonons. The respective amplitudes depend on the excitation level and can be determined by quantum statistical methods. The energy levels of a lattice vibration ($\mathbf{q}, j$) are those of a single harmonic oscillator:

Copyright © 2006 International Union of Crystallography