5.4 Magnetoelastic effects

The magnetoelastic coupling between the magnetic moments and the lattice modifies the spin waves in two different ways. The *static* deformations of the crystal, induced by the ordered moments, introduce new anisotropy terms in the spin-wave Hamiltonian. The *dynamic* time-dependent modulations of the magnetic moments furthermore interfere with the lattice vibrations. We shall start with a discussion of the static effects, and then consider the magnon–phonon interaction. The magnetoelastic crystal-field Hamiltonian was introduced in Section 1.4, where the different contributions were classified according to the symmetry of the strain parameters. The two-ion coupling may also change with the strain, as exemplified by eqn (2.2.32). We shall continue considering the basal-plane ferromagnet and, in order to simplify the discussion, we shall only treat the low-rank magnetoelastic couplings of single-ion origin. In the ferromagnetic case, the magnetoelastic two-ion couplings do not introduce any effects which differ qualitatively from those due to the crystal-field interactions. Consequently, those interactions which are not included in the following discussion only influence the detailed dependence of the effective coupling parameters on the magnetization and, in the case of the dynamics, on the wave-vector.

5.4.1 Magnetoelastic effects on the energy gap

The static effects of the α-strains on the spin-wave energies may be included in a straightforward manner, by replacing the crystal-field parameters in (5.2.1) with effective strain-dependent values, i.e. $B_2^0 \to B_2^0 + B_{\alpha 1}^{(2)}\,\bar{\epsilon}_{\alpha 1} + B_{\alpha 2}^{(2)}\,\bar{\epsilon}_{\alpha 2}$, with α-strains proportional to $\langle Q_2^0 \rangle$. Equivalent contributions appear in the magnetic anisotropy, discussed in Section 2.2.2. This simplification is not possible with the γ- or the ϵ-strain contributions, because these, in contrast to the α-strains, change the symmetry of the lattice. When $\theta = \pi/2$, the ϵ-strains vanish, and the

γ-strain part of the magnetoelastic Hamiltonian is given by eqn (2.2.23):

$$\mathcal{H}_\gamma = \sum_i \big[\tfrac{1}{2}c_\gamma(\epsilon_{\gamma1}^2 + \epsilon_{\gamma2}^2) - B_{\gamma2}\{Q_2^2(\mathbf{J}_i)\epsilon_{\gamma1} + Q_2^{-2}(\mathbf{J}_i)\epsilon_{\gamma2}\} \\ - B_{\gamma4}\{Q_4^4(\mathbf{J}_i)\epsilon_{\gamma1} - Q_4^{-4}(\mathbf{J}_i)\epsilon_{\gamma2}\}\big]. \tag{5.4.1}$$

The equilibrium condition, $\partial F/\partial\epsilon_\gamma = 0$, leads to eqn (2.2.25) for the static strains $\bar{\epsilon}_\gamma$. The static-strain variables are distinguished by a bar from the dynamical contributions $\epsilon_\gamma - \bar{\epsilon}_\gamma$. The expectation values of the Stevens operators may be calculated by the use of the RPA theory developed in the preceding section, and with $\theta = \pi/2$ we obtain, for instance,

$$\langle Q_2^2\rangle = \langle \tfrac{1}{2}(O_2^0 + O_2^2)\cos 2\phi + 2O_2^{-1}\sin 2\phi\rangle = J^{(2)}\hat{I}_{5/2}[\sigma]\eta_-^{-1}\cos 2\phi \\ \langle Q_2^{-2}\rangle = \langle \tfrac{1}{2}(O_2^0 + O_2^2)\sin 2\phi - 2O_2^{-1}\cos 2\phi\rangle = J^{(2)}\hat{I}_{5/2}[\sigma]\eta_-^{-1}\sin 2\phi. \tag{5.4.2}$$

We note that $\langle O_2^{-1}\rangle$ vanishes only as long as $\mathcal{H}'$ in (5.2.12) can be neglected. Introducing the magnetostriction parameters C and A via eqn (2.2.26a), when $\theta = \pi/2$,

$$\bar{\epsilon}_{\gamma1} = C\cos 2\phi - \tfrac{1}{2}A\cos 4\phi \\ \bar{\epsilon}_{\gamma2} = C\sin 2\phi + \tfrac{1}{2}A\sin 4\phi, \tag{5.4.3}$$

and calculating $\langle Q_4^{\pm4}\rangle$, we obtain

$$C = \frac{1}{c_\gamma}B_{\gamma2}J^{(2)}\hat{I}_{5/2}[\sigma]\eta_-^{-1} \\ A = -\frac{2}{c_\gamma}B_{\gamma4}J^{(4)}\hat{I}_{9/2}[\sigma]\eta_-^{-6}, \tag{5.4.4}$$

instead of eqn (2.2.26b), including the effects of the elliptical precession of the moments. The equilibrium conditions allow us to split the magnetoelastic Hamiltonian into two parts:

$$\mathcal{H}_\gamma(\mathrm{sta}) = \sum_i \big[\tfrac{1}{2}c_\gamma(\bar{\epsilon}_{\gamma1}^2 + \bar{\epsilon}_{\gamma2}^2) - B_{\gamma2}\{Q_2^2(\mathbf{J}_i)\bar{\epsilon}_{\gamma1} + Q_2^{-2}(\mathbf{J}_i)\bar{\epsilon}_{\gamma2}\} \\ - B_{\gamma4}\{Q_4^4(\mathbf{J}_i)\bar{\epsilon}_{\gamma1} - Q_4^{-4}(\mathbf{J}_i)\bar{\epsilon}_{\gamma2}\}\big], \tag{5.4.5}$$

depending only on the static strains, and

$$\mathcal{H}_\gamma(\mathrm{dyn}) = \sum_i \Big[\tfrac{1}{2}c_\gamma\{(\epsilon_{\gamma1} - \bar{\epsilon}_{\gamma1})^2 + (\epsilon_{\gamma2} - \bar{\epsilon}_{\gamma2})^2\} \\ - \big(B_{\gamma2}\{Q_2^2(\mathbf{J}_i) - \langle Q_2^2\rangle\} + B_{\gamma4}\{Q_4^4(\mathbf{J}_i) - \langle Q_4^4\rangle\}\big)(\epsilon_{\gamma1} - \bar{\epsilon}_{\gamma1}) \\ - \big(B_{\gamma2}\{Q_2^{-2}(\mathbf{J}_i) - \langle Q_2^{-2}\rangle\} - B_{\gamma4}\{Q_4^{-4}(\mathbf{J}_i) - \langle Q_4^{-4}\rangle\}\big)(\epsilon_{\gamma2} - \bar{\epsilon}_{\gamma2})\Big] \tag{5.4.6}$$

depending only on the dynamical part of the strains.

To leading order, the magnetoelastic energy is determined by the static part (5.4.5), corresponding to eqn (2.2.27). $\mathcal{H}_\gamma$ influences the equilibrium condition determining ϕ and, in the spin-wave approximation ($\mathcal{H}'$ is neglected), we have

$$\begin{aligned}\frac{1}{N}\frac{\partial F}{\partial \phi} &= \frac{1}{N}\Big\langle\frac{\partial}{\partial\phi}\{\mathcal{H}+\mathcal{H}_\gamma\}\Big\rangle \simeq \frac{1}{N}\Big\langle\frac{\partial}{\partial\phi}\{\mathcal{H}+\mathcal{H}_\gamma(\mathrm{sta})\}\Big\rangle \\ &= -\,6B_6^6 J^{(6)}\hat{I}_{13/2}[\sigma]\eta_-^{-15}\sin 6\phi + g\mu_B H J\sigma\sin(\phi-\phi_H) \\ &\quad +2c_\gamma C(\overline{\epsilon}_{\gamma1}\sin 2\phi - \overline{\epsilon}_{\gamma2}\cos 2\phi) - 2c_\gamma A(\overline{\epsilon}_{\gamma1}\sin 4\phi + \overline{\epsilon}_{\gamma2}\cos 4\phi),\end{aligned} \tag{5.4.7}$$

or, using the equilibrium values of $\overline{\epsilon}_{\gamma1}$ and $\overline{\epsilon}_{\gamma2}$,

$$\frac{1}{N}\frac{\partial F}{\partial \phi} = g\mu_B J\sigma\big\{H\sin(\phi-\phi_H) - \tfrac{1}{6}\widetilde{H}_c\sin 6\phi\big\}, \tag{5.4.8a}$$

with the definition

$$g\mu_B\widetilde{H}_c = 36\kappa_6^6/(J\sigma) = 36\big\{B_6^6 J^{(6)}\hat{I}_{13/2}[\sigma]\eta_-^{-15} + \tfrac{1}{2}c_\gamma CA\big\}/(J\sigma). \tag{5.4.8b}$$

If $H = 0$, the equilibrium condition $\partial F/\partial\phi = 0$ determines the stable direction of magnetization to be along either a b-axis or an a-axis, depending on whether $\widetilde{H}_c$ is positive or negative respectively.

The additional anisotropy terms introduced by $\mathcal{H}_\gamma$ and proportional to the static strains, as for instance the term $-B_{\gamma2}Q_2^2(\mathbf{J}_i)\overline{\epsilon}_{\gamma1}$ in (5.4.5), contribute to the spin-wave energies. Proceeding as in Section 5.3, we find the additional contributions to $A_\mathbf{0}(T) \pm B_\mathbf{0}(T)$ in (5.3.22), proportional to the static γ-strains,

$$\begin{aligned}\Delta\{A_\mathbf{0}(T) + B_\mathbf{0}(T)\} &\\ = \frac{c_\gamma}{J\sigma}&\big\{2C^2 + A^2\eta_+^{-8}\eta_-^{-4} - CA(2+\eta_+^{-8}\eta_-^{-4})\cos 6\phi\big\}\eta_+^{-1}\eta_- \\ \Delta\{A_\mathbf{0}(T) - B_\mathbf{0}(T)\} &= \frac{c_\gamma}{J\sigma}\big\{4C^2 + 4A^2 - 10CA\cos 6\phi\big\}.\end{aligned} \tag{5.4.9}$$

The contribution to $A_\mathbf{0}(T) - B_\mathbf{0}(T)$ is expressible directly in terms of the strain-parameters, C and A, without the further correction factors necessary for $A_\mathbf{0}(T)+B_\mathbf{0}(T)$. By using $\widetilde{H}_c$ and the non-negative quantity

$$\Lambda_\gamma = \frac{4c_\gamma}{J\sigma}(C^2 + A^2 + 2CA\cos 6\phi), \tag{5.4.10}$$

we can write the *total* spin-wave parameter

$$A_\mathbf{0}(T) - B_\mathbf{0}(T) = \Lambda_\gamma - g\mu_B\widetilde{H}_c\cos 6\phi + g\mu_B H\cos(\phi-\phi_H). \tag{5.4.11}$$

This parameter does not obey the relation (5.3.14) with the second derivative $F_{\phi\phi}$ of the free energy. A differentiation $\partial F/\partial\phi$, as given by (5.4.8), with respect to ϕ shows that (5.3.14) accounts for the last two terms in (5.4.11), but not for Λ_γ. A calculation from (5.4.7) of the second derivative of F, when the strains are kept constant, instead of under the constant (zero) stress-condition assumed above, yields

$$A_{\mathbf{0}}(T) - B_{\mathbf{0}}(T) = \frac{1}{NJ\sigma}\frac{\partial^2 F}{\partial\phi^2}\bigg|_{\epsilon=\overline{\epsilon}} = \Lambda_\gamma + \frac{1}{NJ\sigma}F_{\phi\phi}, \tag{5.4.12}$$

which replaces (5.3.14). The relation (5.3.14), determining $A_{\mathbf{0}}(T) - B_{\mathbf{0}}(T)$, was based on a calculation of the frequency dependence of the bulk susceptibility and, as we shall see later, it is the influence of the lattice which invalidates this argument. The Λ_γ term was originally suggested by Turov and Shavrov (1965), who called it the 'frozen lattice' contribution because the dynamic strain-contributions were not considered. However, as we shall show in the next section, the magnon–phonon coupling does not change this result.

The modifications caused by the magnetoelastic γ-strain couplings are strongly accentuated at a second-order phase transition, at which $F_{\phi\phi}$ vanishes. Let us consider the case where $\widetilde{H}_c$ is positive, $\widetilde{H}_c = |\widetilde{H}_c| \equiv H_c$, i.e. the b-axis is the easy axis. If a field is applied along an a-axis, $\phi_H = 0$, then the magnetization is pulled towards this direction, as described by eqn (5.4.8):

$$H = H_c\,\frac{\sin 6\phi}{6\sin\phi} = H_c\big(1 - \tfrac{16}{3}\sin^2\phi + \tfrac{16}{3}\sin^4\phi\big)\cos\phi, \tag{5.4.13}$$

as long as the field is smaller than H_c. At the critical field $H = H_c$, the moments are pulled into the hard direction, so that $\phi = 0$ and the second derivative of the free energy,

$$F_{\phi\phi} = Ng\mu_B\{H\cos\phi - H_c\cos 6\phi\}J\sigma, \tag{5.4.14}$$

vanishes. So a second-order phase transition occurs at $H = H_c$, and the order parameter can be considered to be the component of the moments perpendicular to the a-axis, which is zero for $H \geq H_c$. An equally good choice for the order parameter is the strain $\overline{\epsilon}_{\gamma 2}$, and these two possibilities reflect the nature of the linearly coupled magnetic–structural phase transition. The free energy does not contain terms which are cubic in the order parameters, but the transition might be changed into one of first-order by terms proportional to $\cos 12\phi$, e.g. if σ or $\eta_\pm$, and thereby $\widetilde{H}_c$, depend sufficiently strongly on ϕ (Jensen 1975). At the transition, eqn (5.4.11) leads to

$$A_{\mathbf{0}}(T) - B_{\mathbf{0}}(T) = \Lambda_\gamma \qquad \text{at} \quad H = H_c, \tag{5.4.15}$$

which shows the importance of the constant-strain contribution Λ_γ. It ensures that the spin-wave energy gap $E_{\mathbf{0}}(T)$, instead of going to zero as $|H - H_c|^{1/2}$, remains non-zero, as illustrated in Fig. 5.4, when the transition at $H = H_c$ is approached. Such a field just cancels the macroscopic hexagonal anisotropy, but energy is still required in the spin wave to precess the moments against the strain field of the lattice.

By symmetry, the γ-strains do not contain terms linear in $(\theta - \frac{\pi}{2})$, and the choice between constant-stress and constant-strain conditions therefore has no influence on their contribution to the second derivative of F with respect to θ, at $\theta = \pi/2$. Consequently, the γ-strains do not change the relation between $A_{\mathbf{0}}(T) + B_{\mathbf{0}}(T)$ and $F_{\theta\theta}$, given by eqn (5.3.14). The ε-strains vanish at $\theta = \pi/2$, but they enter linearly with $(\theta - \frac{\pi}{2})$. Therefore they have no effect on $A_{\mathbf{0}}(T) + B_{\mathbf{0}}(T)$, but they contribute to $F_{\theta\theta}$. To see this, we consider the ε-strain part of the Hamiltonian, eqn (2.2.29):

$$\mathcal{H}_\varepsilon = \sum_i \left[\tfrac{1}{2} c_\varepsilon (\epsilon_{\varepsilon 1}^2 + \epsilon_{\varepsilon 2}^2) - B_{\varepsilon 1}\{Q_2^1(\mathbf{J}_i)\epsilon_{\varepsilon 1} + Q_2^{-1}(\mathbf{J}_i)\epsilon_{\varepsilon 2}\}\right]. \qquad (5.4.16)$$

The equilibrium condition is

$$\overline{\epsilon}_{\varepsilon 1} = \frac{1}{c_\varepsilon} B_{\varepsilon 1} \langle Q_2^1 \rangle = \tfrac{1}{4} H_\varepsilon \sin 2\theta \cos\phi,$$

in terms of the magnetostriction parameter H_ε. In the basal-plane ferromagnet, $\overline{\epsilon}_{\varepsilon 1}$ and $\overline{\epsilon}_{\varepsilon 2}$ both vanish. The transformation (5.2.2) leads to

$$Q_2^1 = \tfrac{1}{4}(O_2^0 - O_2^2) \sin 2\theta \cos\phi - O_2^1 \cos 2\theta \cos\phi + O_2^{-1} \cos\theta \sin\phi + \tfrac{1}{2} O_2^{-2} \sin\theta \sin\phi, \qquad (5.4.17)$$

and Q_2^{-1} is given by the same expression, if ϕ is replaced by $\phi - \frac{\pi}{2}$. This implies that

$$H_\varepsilon = \frac{4}{c_\varepsilon} B_{\varepsilon 1} \langle \tfrac{1}{4}(O_2^0 - O_2^2) \rangle = \frac{2}{c_\varepsilon} B_{\varepsilon 1} J^{(2)} \hat{I}_{5/2}[\sigma] \eta_+^{-1}. \qquad (5.4.18)$$

The static ε-strains are zero and do not contribute to the spin-wave parameters $A_{\mathbf{0}}(T) \pm B_{\mathbf{0}}(T)$, but they affect the second derivative of F, with respect to θ, under zero-stress conditions and, corresponding to (5.4.12), we have

$$A_{\mathbf{0}}(T) + B_{\mathbf{0}}(T) = \frac{1}{NJ\sigma} \frac{\partial^2 F}{\partial \theta^2}\bigg|_{\epsilon = \overline{\epsilon}} = \Lambda_\varepsilon + \frac{1}{NJ\sigma} F_{\theta\theta}, \qquad (5.4.19)$$

with

$$\Lambda_\varepsilon = \frac{c_\varepsilon}{4J\sigma} H_\varepsilon^2, \tag{5.4.20}$$

where Λ_ε in (5.4.19) just cancels the ε-contribution to $F_{\theta\theta}/(NJ\sigma)$ determined from eqn (2.2.34).

The dependence of the magnon energy gap in Tb on magnetic field and temperature has been studied in great detail by Houmann *et al.* (1975a). They expressed the axial- and hexagonal-anisotropy energies of eqn (5.2.44) in the form

$$A_0(T) \pm B_0(T) = P_0(\pm) - P_6(\pm)\cos 6\phi + g\mu_B H \cos(\phi - \phi_H) \tag{5.4.21}$$

and, by a least-squares fitting of their results, some of which are shown in Fig. 5.4, they were able to deduce the values of the four parameters $P_{0,6}(\pm)$, shown as a function of magnetization in Fig. 5.5. According to eqns (5.3.22) and (5.4.9), these parameters are given at low temperatures by:

$$P_0(+) = \{6B_2^0 J^{(2)} - 60B_4^0 J^{(4)} + 210B_6^0 J^{(6)} + c_\gamma(2C^2 + A^2)\}/J \quad (a)$$
$$P_6(+) = \{6B_6^6 J^{(6)} + 3c_\gamma CA\}/J \quad (b)$$
$$P_0(-) = 4c_\gamma\{C^2 + A^2\}/J \quad (c)$$
$$P_6(-) = \{36B_6^6 J^{(6)} + 10c_\gamma CA\}/J, \quad (d)$$
$$(5.4.22)$$

where, for convenience, we have set the renormalization parameters σ and $\eta_\pm$ to unity. These expressions for the parameters $P_{0,6}(\pm)$ are derived from a particular model. In general, additional contributions may appear due to other magnetoelastic interactions, and to anisotropic two-ion couplings. Nevertheless, within the RPA, the relations between the spin-wave energy parameters $A_{\mathbf{0}}(T) \pm B_{\mathbf{0}}(T)$ and the bulk anisotropy parameters, (5.4.12) and (5.4.19) combined with (5.3.7), should still be valid. The values of the anisotropy parameters, and their temperature dependences, determine the static magnetic and magnetoelastic properties, and can thus be obtained from bulk measurements on single crystals. A comparison between such static parameters and the dynamic values $P_{0,6}(\pm)$, derived from the field dependence of the spin-wave energy gap, can therefore elucidate the extent to which the spin-wave theory of the anisotropic ferromagnet is complete and correct.

Such a comparison has been made by Houmann *et al.* (1975a). The axial-anisotropy parameter $P_0(+) + P_6(+)$, when the moments are along the easy axis, agrees with the values deduced from torque and magnetization experiments, to within the rather large uncertainties of the

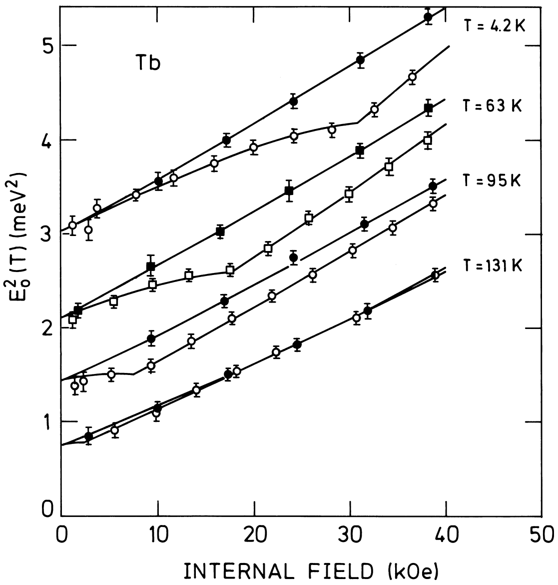

Fig. 5.4. The dependence of the square of the magnon energy gap in Tb on the internal magnetic field. Open symbols represent results for the field in the hard direction, and closed symbols are for the easy direction. The non-zero value of the gap at the critical field, which just turns the moments into the hard direction, is due to the constant-strain contribution Λ_γ. The full lines are least-squares fits of the theoretical expressions for the energy gap, given in the text, to the experimental results.

latter. The basal-plane anisotropies, as determined from the critical field H_c and the magnetoelastic γ-strain parameters, are well established by bulk measurements. Here $P_0(-)$ agrees, within the small combined uncertainties, with that derived from (5.4.22*c*) and (5.4.11), both in magnitude and temperature dependence. On the other hand, the small parameter $P_6(-)$ differs from the static value, so that

$$\delta_6(-) \equiv P_6(-) - g\mu_B \widetilde{H}_c + 8c_\gamma CA/(J\sigma) \qquad (5.4.23a)$$

is found to be non-zero. A part of this discrepancy may be explained by a twelve-fold anisotropy term, but this would also affect $P_0(-)$, and is expected to decrease more rapidly with increasing temperature than the experiments indicate. Within the accuracy of the experimental results, the non-zero value of $\delta_6(-)$ is the only indication of an additional renormalization of the spin-wave energy gap, compared with that derived from the second derivatives of the free energy.

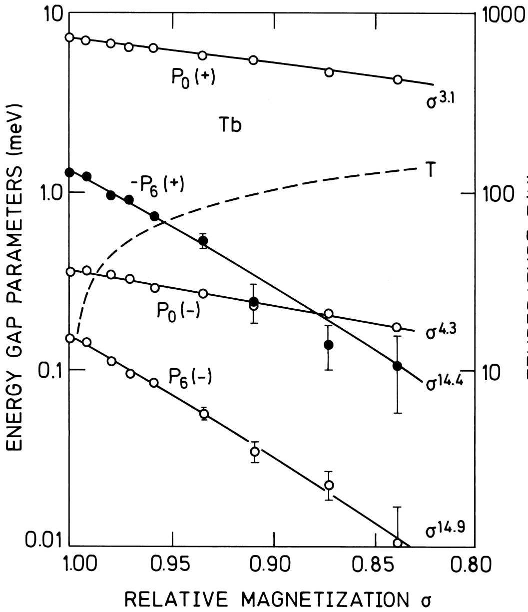

Fig. 5.5. Anisotropy parameters in Tb as a function of the relative magnetization, deduced from results of the type illustrated in Fig. 5.4.

The σ^3-dependence of $P_0(+)$ on temperature is consistent with the σ^2-renormalization of the dominant two-fold term in (5.4.22a) predicted by the Callen–Callen theory, but a comparison with the studies of dilute Tb-alloys by Høg and Touborg (1975) suggests that a large part of the axial anisotropy may have its origin in the two-ion coupling. The effect of the two-ion anisotropy is directly apparent in that part of the axial anisotropy $P_6(+)$ which depends on the orientation of the moments in the basal plane. If only single-ion anisotropy of the type which we have considered is important, $P_6(+)$ in (5.4.22b) is directly related to the critical field necessary to turn the moments into the hard direction. However, the experimental value of $P_6(+)$ bears little relation to $g\mu_B\widetilde{H}_c/6$, even having the opposite sign. We can express this discrepancy by the parameter ΔM, defined by

$$\Delta M = P_6(+) - g\mu_B\widetilde{H}_c/6. \qquad (5.4.23b)$$

The influence of ΔM can be directly seen in the results of Fig. 5.4, since it is responsible for the difference between the slopes when the field is applied in the easy and hard directions. Although it could in principle be due to higher-rank γ-strain magnetoelastic terms, the large magnitude of ΔM, compared to the contributions of C and A to the energy gap, effectively precludes this possibly. We must therefore ascribe it to two-ion anisotropy.

In the analysis of the field dependence of the magnon energy gap, the possible dependences of the renormalization parameters σ and $\eta_\pm$ on magnetic field and the orientation of the moments were neglected at zero temperature, but included at non-zero temperatures, assuming the different parameters effectively to be functions of σ only. In the case of Dy, the zero-temperature change of the renormalization as a function of ϕ is of some importance (Egami 1972; Jensen 1975; Egami and Flanders 1976), whereas in Tb we have estimated by various means that both approximations are justified. There are some indications that there might be a systematic error involved in the determination of the ϕ-dependent energy-gap parameters $P_6(\pm)$, possibly arising from the influence of the classical dipole forces on the inelastic neutron-scattering at long wavelength, discussed in Section 5.5.1. An extrapolation of the results found at non-zero wave-vectors to $\mathbf{q} = \mathbf{0}$ suggests that both $P_6(+)$ and $P_6(-)$ may be about a factor of two smaller than shown in Fig. 5.5. If this were the case, ΔM would still be too large to be explained by the γ-strain couplings, but $\delta_6(-)$ would be reduced almost to the level of the experimental uncertainties. Otherwise a non-zero value of $\delta_6(-)$ can only be explained by theories beyond the RPA, e.g. by effects, proportional to the frequency, due to the interaction between the spin-waves and the electron-hole pair-excitations of the conduction electrons.

5.4.2 The magnon–phonon interaction

The displacement of the ith ion from its equilibrium position, $\delta\mathbf{R}_i = \mathbf{u}(\mathbf{R}_i)$, can be expanded in normal phonon coordinates in the usual way:

$$\mathbf{u}(\mathbf{R}_i) = \sum_{\nu\mathbf{k}} \mathbf{F}^{\nu}_{\mathbf{k}}(\beta_{\nu\mathbf{k}} + \beta^{+}_{\nu-\mathbf{k}})e^{i\mathbf{k}\cdot\mathbf{R}_i}, \tag{5.4.24a}$$

with

$$F^{\nu}_{\mathbf{k},\alpha} = \left[\frac{\hbar}{2NM\omega_{\nu\mathbf{k}}}\right]^{\frac{1}{2}} f^{\nu}_{\mathbf{k},\alpha}. \tag{5.4.24b}$$

M is the mass of the ions and $f^{\nu}_{\mathbf{k},\alpha}$ is the α-component of the phonon-polarization vector. $\beta_{\nu\mathbf{k}}$ is the phonon-annihilation operator and $\omega_{\nu\mathbf{k}}$ the corresponding phonon frequency, where ν denotes one of the three (acoustic) branches. The polarization vectors are normalized and are mutually orthogonal:

$$\sum_{\alpha}(f^{\nu}_{\mathbf{k},\alpha})^* f^{\nu'}_{\mathbf{k},\alpha} = \delta_{\nu\nu'}. \tag{5.4.24c}$$

For simplicity, we assume that there is only one ion per unit cell, but the results we shall derive are also applicable to the hcp lattice, at least for the acoustic modes at long wavelengths. In this limit $\mathcal{H}_\gamma(\text{dyn})$, eqn (5.4.6), augmented by the kinetic energy of the ions, is adequate for discussing dynamical effects due to the γ-strains, if $\epsilon_{\alpha\beta}$ are replaced by their local values

$$\epsilon_{\alpha\beta}(i) = \overline{\epsilon}_{\alpha\beta} + \frac{i}{2}\sum_{\nu\mathbf{k}}(k_\alpha F^\nu_{\mathbf{k},\beta} + k_\beta F^\nu_{\mathbf{k},\alpha})(\beta_{\nu\mathbf{k}} + \beta^+_{\nu-\mathbf{k}})e^{i\mathbf{k}\cdot\mathbf{R}_i}. \qquad (5.4.25)$$

We shall initially concentrate on the most important dynamical effects, and consider only the inhomogeneous-strain terms involving Stevens operators with odd m. Assuming for the moment that $\phi = p\frac{\pi}{2}$, we obtain the contribution $-B_{\gamma2}\{-2O_2^{-1}(\mathbf{J}_i)\cos 2\phi\}(\epsilon_{\gamma2}(i) - \overline{\epsilon}_{\gamma2})$ from eqn (5.4.6), and a corresponding term in $B_{\gamma4}$. Introducing the spin-deviation operators through (5.2.8) and (5.2.9), we obtain, to leading order in m and b,

$$\begin{aligned} B_{\gamma2}O_2^{-1}(\mathbf{J}_i) &= J^{(2)}B_{\gamma2}\frac{i}{\sqrt{2J}}\big\{a_i^+ - a_i - \frac{5}{4J}(a_i^+a_i^+a_i - a_i^+a_ia_i)\big\} \\ &= J^{(2)}B_{\gamma2}\frac{i}{\sqrt{2J}}\big(1 - \tfrac{5}{2}m + \tfrac{5}{4}b\big)(a_i^+ - a_i) \\ &= c_\gamma C\frac{i}{\sqrt{2J}}\big(1 + \tfrac{1}{2}m + \tfrac{1}{4}b\big)(a_i^+ - a_i) \\ &= ic_\gamma C\sum_{\mathbf{q}}\left[\frac{A_{\mathbf{q}}(T) + B_{\mathbf{q}}(T)}{2NJ\sigma E_{\mathbf{q}}(T)}\right]^{\frac{1}{2}}(\alpha^+_{\mathbf{q}} - \alpha_{-\mathbf{q}})\,e^{-i\mathbf{q}\cdot\mathbf{R}_i}, \end{aligned} \qquad (5.4.26)$$

utilizing the RPA decoupling (5.2.29) and introducing the (renormalized) magnon operators $\alpha^+_{\mathbf{q}}$ and $\alpha_{-\mathbf{q}}$, analogously with (5.2.39) and (5.2.40). The $B_{\gamma4}$-term is treated in the same way, and introducing the phonon-operator expansion of the strains (5.4.25) into (5.4.6), we find that $\mathcal{H} + \mathcal{H}_\gamma$ leads to the following Hamiltonian for the system of magnons and phonons:

$$\mathcal{H}_{\text{mp}} = \sum_{\mathbf{k}} E_{\mathbf{k}}(T)\alpha^+_{\mathbf{k}}\alpha_{\mathbf{k}} + \sum_{\nu\mathbf{k}}\big\{\hbar\omega_{\nu\mathbf{k}}\beta^+_{\nu\mathbf{k}}\beta_{\nu\mathbf{k}} + W^\nu_{\mathbf{k}}(\alpha^+_{\mathbf{k}} - \alpha_{-\mathbf{k}})(\beta_{\nu\mathbf{k}} + \beta^+_{\nu-\mathbf{k}})\big\} \qquad (5.4.27)$$

with a *magnon–phonon interaction* given by

$$W^\nu_{\mathbf{k}} = -c_\gamma\sqrt{N}(k_1F^\nu_{\mathbf{k},2} + k_2F^\nu_{\mathbf{k},1})\left[\frac{A_{\mathbf{k}}(T) + B_{\mathbf{k}}(T)}{2J\sigma E_{\mathbf{k}}(T)}\right]^{\frac{1}{2}}(C\cos 2\phi + A\cos 4\phi). \qquad (5.4.28)$$

This Hamiltonian includes the part of $\mathcal{H}_\gamma$ which is linear in the magnon operators when $\phi = p\frac{\pi}{2}$. The effects of the static deformations are included in $E_{\mathbf{k}}(T)$ through (5.4.11). In general, $W^{\nu}_{\mathbf{k}}$ couples all three phonon modes with the magnons. A simplification occurs when $\mathbf{k}$ is along the 1- or 2-axis, i.e. when $\mathbf{k}$ is either parallel or perpendicular to the magnetization vector. In this case, $W^{\nu}_{\mathbf{k}}$ is only different from zero when ν specifies the mode as a transverse phonon with its polarization vector parallel to the basal plane. In order to analyse this situation, we introduce the four Green functions:

$$\begin{aligned} G_1(\mathbf{k},\omega) &= \langle\langle \alpha_{\mathbf{k}}\,;\,\alpha^+_{\mathbf{k}} - \alpha_{-\mathbf{k}}\rangle\rangle \qquad G_2(\mathbf{k},\omega) = \langle\langle \alpha^+_{-\mathbf{k}}\,;\,\alpha^+_{\mathbf{k}} - \alpha_{-\mathbf{k}}\rangle\rangle \\ G_3(\mathbf{k},\omega) &= \langle\langle \beta_{\mathbf{k}}\,;\,\alpha^+_{\mathbf{k}} - \alpha_{-\mathbf{k}}\rangle\rangle \qquad G_4(\mathbf{k},\omega) = \langle\langle \beta^+_{-\mathbf{k}}\,;\,\alpha^+_{\mathbf{k}} - \alpha_{-\mathbf{k}}\rangle\rangle, \end{aligned} \tag{5.4.29}$$

where the phonon mode is as specified above (the index ν is suppressed). $\mathcal{H}_{\rm mp}$ then leads to the following coupled equations of motion for these Green functions:

$$\begin{aligned} &\{\hbar\omega - E_{\mathbf{k}}(T)\}G_1(\mathbf{k},\omega) - W_{\mathbf{k}}\{G_3(\mathbf{k},\omega) + G_4(\mathbf{k},\omega)\} = 1 \\ &\{\hbar\omega + E_{\mathbf{k}}(T)\}G_2(\mathbf{k},\omega) - W_{\mathbf{k}}\{G_3(\mathbf{k},\omega) + G_4(\mathbf{k},\omega)\} = 1 \\ &\{\hbar\omega - \hbar\omega_{\mathbf{k}}\}G_3(\mathbf{k},\omega) + W_{-\mathbf{k}}\{G_1(\mathbf{k},\omega) - G_2(\mathbf{k},\omega)\} = 0 \\ &\{\hbar\omega + \hbar\omega_{\mathbf{k}}\}G_4(\mathbf{k},\omega) - W_{-\mathbf{k}}\{G_1(\mathbf{k},\omega) - G_2(\mathbf{k},\omega)\} = 0. \end{aligned} \tag{5.4.30}$$

These four equations may be solved straightforwardly and, using $W_{-\mathbf{k}} = -W_{\mathbf{k}}$, we obtain, for instance,

$$\begin{aligned} \langle\langle \alpha_{\mathbf{k}} - \alpha^+_{-\mathbf{k}}\,;\,\alpha^+_{\mathbf{k}} - \alpha_{-\mathbf{k}}\rangle\rangle &= G_1(\mathbf{k},\omega) - G_2(\mathbf{k},\omega) \\ &= 2E_{\mathbf{k}}(T)\{(\hbar\omega)^2 - (\hbar\omega_{\mathbf{k}})^2\}/\mathcal{D}(\mathbf{k},\omega), \end{aligned} \tag{5.4.31}$$

where the denominator is

$$\mathcal{D}(\mathbf{k},\omega) = \{(\hbar\omega)^2 - E^2_{\mathbf{k}}(T)\}\{(\hbar\omega)^2 - (\hbar\omega_{\mathbf{k}})^2\} - 4W^2_{\mathbf{k}}\hbar\omega_{\mathbf{k}}E_{\mathbf{k}}(T). \tag{5.4.32}$$

In a similar way, introducing the appropriate Green functions, we find

$$\langle\langle \alpha_{\mathbf{k}} + \alpha^+_{-\mathbf{k}}\,;\,\alpha^+_{\mathbf{k}} + \alpha_{-\mathbf{k}}\rangle\rangle = \big[2E_{\mathbf{k}}(T)\{(\hbar\omega)^2 - (\hbar\omega_{\mathbf{k}})^2\} + 8W^2_{\mathbf{k}}\hbar\omega_{\mathbf{k}}\big]/\mathcal{D}(\mathbf{k},\omega). \tag{5.4.33}$$

In this situation, the polarization factor is $(k_1 f_{\mathbf{k},2} + k_2 f_{\mathbf{k},1}) = \pm k$, with $k = |\mathbf{k}|$. At long wavelengths, the velocity $v = \omega_{\mathbf{k}}/k$ of the transverse sound waves is related to the elastic constant $c_{66} = \rho v^2$, and hence

$$c_\gamma = 4c_{66}V/N = 4M\omega^2_{\mathbf{k}}/k^2, \tag{5.4.34}$$

and the coupling term in $\mathcal{D}(\mathbf{k},\omega)$ can be written

$$4W^2_{\mathbf{k}}\hbar\omega_{\mathbf{k}}E_{\mathbf{k}}(T) = \{A_{\mathbf{k}}(T) + B_{\mathbf{k}}(T)\}(\hbar\omega_{\mathbf{k}})^2\Lambda_\gamma, \tag{5.4.35}$$

where the parameter Λ_γ is given by (5.4.10). The magnetic susceptibilities can be expressed in terms of the Green functions calculated above, using (5.2.39) and (5.2.40), and we finally arrive at

$$\chi_{xx}(\mathbf{q},\omega) = J\sigma\big[\{A_{\mathbf{q}}(T) - B_{\mathbf{q}}(T)\}\{(\hbar\omega_{\mathbf{q}})^2 - (\hbar\omega)^2\} - \Lambda_\gamma(\hbar\omega_{\mathbf{q}})^2\big]/\mathcal{D}(\mathbf{q},\omega) \tag{5.4.36a}$$

and

$$\chi_{yy}(\mathbf{q},\omega) = J\sigma\{A_{\mathbf{q}}(T) + B_{\mathbf{q}}(T)\}\{(\hbar\omega_{\mathbf{q}})^2 - (\hbar\omega)^2\}/\mathcal{D}(\mathbf{q},\omega). \tag{5.4.36b}$$

Because $\omega_{\mathbf{q}} \propto q$ and $E_{\mathbf{0}}(T) > 0$, it is possible to satisfy the inequality $E_{\mathbf{q}}(T) \gg \hbar\omega_{\mathbf{q}}$ by choosing a sufficiently small q. As mentioned earlier, $E_{\mathbf{0}}(T)$ is always greater than zero, if the magnetoelastic coupling is non-zero, on account of the constant-strain term Λ_γ. Under these circumstances the elementary-excitation energies, determined by the poles of the susceptibilities or by $\mathcal{D}(\mathbf{q},\omega) = 0$, are found to be

$$(\hbar\omega)^2 = \begin{cases} E_{\mathbf{q}}^2(T) + 4W_{\mathbf{q}}^2\hbar\omega_{\mathbf{q}}/E_{\mathbf{q}}(T) \\ (\hbar\omega_{\mathbf{q}})^2 - 4W_{\mathbf{q}}^2\hbar\omega_{\mathbf{q}}/E_{\mathbf{q}}(T), \end{cases} \tag{5.4.37}$$

to leading order in $\hbar\omega_{\mathbf{q}}/E_{\mathbf{q}}(T)$. The different excitations have become mixed magnetoelastic modes, which mutually repel due to the magnetoelastic coupling, and their squared energies are shifted up or down by an equal amount. When $E_{\mathbf{q}}(T) \gg \hbar\omega_{\mathbf{q}}$, the change in energy of the upper, predominantly magnon-like branch can be neglected, whereas the frequency of the lower phonon-like mode, as obtained from (5.4.37), using the relation (5.4.35),

$$\omega^2 = \omega_{\mathbf{q}}^2\left(1 - \frac{\Lambda_\gamma}{A_{\mathbf{0}}(T) - B_{\mathbf{0}}(T)}\right) + \mathcal{O}\big(\{\hbar\omega_{\mathbf{q}}/E_{\mathbf{q}}(T)\}^4\big), \tag{5.4.38a}$$

may be modified appreciably relative to the unperturbed phonon frequency. This relation implies that the elastic constant, relative to the unperturbed value, as determined by the velocity of these magneto-acoustic sound waves, is

$$\frac{c_{66}^*}{c_{66}} = 1 - \frac{\Lambda_\gamma}{A_{\mathbf{0}}(T) - B_{\mathbf{0}}(T)} \qquad ; \quad \mathbf{q} \parallel \text{ or } \perp \langle \mathbf{J} \rangle. \tag{5.4.38b}$$

At $\mathbf{q} = \mathbf{0}$, the dynamic coupling vanishes identically and the spin-wave energy gap is still found at $\hbar\omega = E_{\mathbf{0}}(T) = \{A_{\mathbf{0}}^2(T) - B_{\mathbf{0}}^2(T)\}^{1/2}$, with the static-strain contributions included in $A_{\mathbf{0}}(T) \pm B_{\mathbf{0}}(T)$. Due to the vanishing of the eigenfrequencies of the elastic waves at zero wave-vector, the lattice cannot respond to a uniform precession of the magnetic moments at a non-zero frequency. Therefore the spin-wave mode at $\mathbf{q} = \mathbf{0}$ perceives the lattice as being completely static or 'frozen'. This is clearly consistent with the result (5.4.12), that the spin-wave energy gap is proportional to the second derivative of the free energy under constant-strain, rather than constant-stress, conditions.

If the lattice is able to adapt itself to the applied constant-stress condition, in the static limit $\omega \ll \omega_{\mathbf{q}}$, then, according to (5.4.36*b*),

$$\chi_{yy}(\mathbf{q} \to \mathbf{0}, 0) = \chi_{yy}(\mathbf{q} \equiv \mathbf{0}, 0) = \frac{J\sigma}{A_{\mathbf{0}}(T) - B_{\mathbf{0}}(T) - \Lambda_\gamma} = N\frac{(J\sigma)^2}{F_{\phi\phi}}, \tag{5.4.39}$$

in agreement with (5.3.7). However, the first equality is not generally valid. The susceptibility depends on the direction from which $\mathbf{q}$ approaches $\mathbf{0}$. If the direction of $\mathbf{q}$ is specified by the spherical coordinates $(\theta_{\mathbf{q}}, \phi_{\mathbf{q}})$, then eqn (5.4.39) is valid only in the configuration considered, i.e. for $\theta_{\mathbf{q}} = \frac{\pi}{2}$ and $\phi_{\mathbf{q}} = 0$ or $\frac{\pi}{2}$. If we assume elastically isotropic conditions ($c_{11} = c_{33}$, $c_{44} = c_{66}$, and $c_{12} = c_{13}$), which is a reasonable approximation in Tb and Dy, we find that (5.4.39) is replaced by the more general result

$$\chi_{yy}(\mathbf{q} \to \mathbf{0}, 0) = \frac{J\sigma}{A_{\mathbf{0}}(T) - B_{\mathbf{0}}(T) - \Lambda_\gamma \sin^2\theta_{\mathbf{q}}\{1 - (1-\xi)\sin^2\theta_{\mathbf{q}}\sin^2 2\phi_{\mathbf{q}}\}}, \tag{5.4.40}$$

when $\phi = 0$ or $\frac{\pi}{2}$, and $\xi = c_{66}/c_{11}$ ($\simeq 0.3$ in Tb or Dy). The reason for this modification is that discussed in Section 2.2.2; the ability of the lattice to adapt to various static-strain configurations is limited if these strains are spatially modulated. If $\mathbf{q}$ is along the c-axis ($\theta_{\mathbf{q}} = 0$), the γ-strains are 'clamped', remaining constant throughout the crystal, so that the susceptibilities at both zero and finite frequencies are determined by the uniform γ-strain contributions alone. We note that, according to (5.4.28), $W_{\mathbf{k}}^{\nu}$ vanishes if $\mathbf{k}$ is parallel to the c-axis ($k_1 = k_2 = 0$). The opposite extreme occurs when $\theta_{\mathbf{q}} = \frac{\pi}{2}$ and $\phi_{\mathbf{q}} = 0$ or $\frac{\pi}{2}$. The relevant strain-mode is determined by the equilibrium conditions (5.4.3) at zero constant stress, but generalized to the non-uniform case where the y-component of the moments has a small modulation, with the wave-vector $\mathbf{q}$ along the x-direction. This strain mode $(\bar{\epsilon}_{\gamma 2}(i) + \overline{\omega}_{21}(i) \propto \cos(\mathbf{q} \cdot \mathbf{R}_i + \varphi))$ coincides with a phonon eigenstate, the transverse phonon at $\mathbf{q}$ with its polarization vector in the basal plane. This coincidence makes the equilibrium strain-mode viable, which then explains the constant-stress result (5.4.39) obtained for χ_{yy} in this situation.

We shall now return to the discussion of the second-order transition occurring at $H = H_c$, when the field is applied along a hard direction in the basal plane. From (5.4.36a), we see that $\chi_{xx}(\mathbf{q} \to \mathbf{0}, 0)$ does not show an anomaly at the transition. The critical behaviour is confined to the yy-component of the static susceptibility. At the transition, $A_{\mathbf{0}}(T) - B_{\mathbf{0}}(T) = \Lambda_\gamma$, according to eqn (5.4.15), and (5.4.40) then predicts a very rapid variation of $\chi_{yy}(\mathbf{q} \to \mathbf{0}, 0)$ with the direction of $\mathbf{q}$, with a divergent susceptibility in the long wavelength limit in the two cases where $\mathbf{q}$ is along the z- or the y-axis, both lying in the basal plane, parallel or perpendicular to the magnetic moments. These divergences reflect a softening of two modes in the system, the transverse phonons propagating parallel to either of the two axes ($\theta_{\mathbf{q}} = \frac{\pi}{2}$ and $\phi_{\mathbf{q}} = p\frac{\pi}{2}$), with their polarization vectors in the basal plane. Equation (5.4.38) predicts that the velocity of these modes is zero, or $c^*_{66} = 0$, at $H = H_c$, at which field the dispersion is quadratic in q instead of being linear. The softening of these modes was clearly observed in the ultrasonic measurements of Jensen and Palmer (1979). Although the ultrasonic velocity could not be measured as a function of magnetic field all the way to H_c, because of the concomitant increase in the attenuation of the sound waves, the mode with $\mathbf{q}$ parallel to the magnetization could be observed softening according to (5.4.38b), until the elastic constant was roughly halved. On the other hand, as discussed in the next section, the dipolar interaction prevents the velocity of the mode in which the ionic motion is along the magnetization from falling to zero, and (5.4.38b) is replaced by (5.5.13). When they took this effect into account, Jensen and Palmer (1979) could fit their results over a wide range of fields and temperatures with the RPA theory, without adjustable parameters or corrections for critical phenomena, using the bulk values of the three basal-plane anisotropy parameters C, A, and $\widetilde{H}_c$,

The absence of such corrections may be explained by the behaviour of the *critical fluctuations*, which is the same as that found in a pure structural phase-transition in an orthorhombic crystal, where c_{66} is again the soft elastic constant (Cowley 1976; Folk *et al.* 1979). The strong bounds set by the geometry on the soft modes in reciprocal space constrain the transition to exhibit mean-field behaviour. The *marginal dimensionality* d^*, as estimated for example by Als-Nielsen and Birgeneau (1977), using a real space version of the Ginzburg criterion, is $d^* = 2$ in this kind of system. Whenever the dimensionality d of the system is larger than d^*, as in this case, Wilson's *renormalization group* theory predicts no corrections to Landau's mean-field theory. The transition at $H = H_c$ is thus profoundly influenced by the magnetoelastic effects. Without them, i.e. with $C = A = 0$, the spin-wave energy gap would vanish at the transition, and the critical fluctuations, the long-wavelength magnons, would not be limited to certain directions in $\mathbf{q}$-space. Under such circumstances, the system would behave analogously to a threedimensional Ising model, $d^* = 4$, with pronounced modifications induced by the critical fluctuations. The original treatment by Turov and Shavrov (1965) of the γ-strain contributions, which prevent the uniform magnon mode from going soft at the critical field, included only the static-strain components. The more complete analyses, including the phonon dynamics, were later given by Jensen (1971a,b), Liu (1972b), and Chow and Keffer (1973).

When the wave-vector is in the c-direction, the γ-strain couplings vanish, but instead the ε-strains become important. The O_2^1-term in Q_2^1, given by eqn (5.4.17), leads to a linear coupling between the magnons and the phonons, and proceeding as in eqns (5.4.26–27), we find the additional contribution to $\mathcal{H}_{\rm mp}$

$$\Delta\mathcal{H}_{\rm mp} = \sum_{\mathbf{k}} iW_{\mathbf{k}}^{\nu}(\varepsilon)(\alpha_{\mathbf{k}}^{+} + \alpha_{-\mathbf{k}})(\beta_{\nu\mathbf{k}} + \beta_{\nu-\mathbf{k}}^{+}), \tag{5.4.41a}$$

with

$$W_{\mathbf{k}}^{\nu}(\varepsilon) = -\tfrac{1}{4}c_{\varepsilon}\sqrt{N}\big\{(k_1F_{\mathbf{k},3}^{\nu} + k_3F_{\mathbf{k},1}^{\nu})\cos\phi + (k_2F_{\mathbf{k},3}^{\nu} + k_3F_{\mathbf{k},2}^{\nu})\sin\phi\big\} \times \left[\frac{A_{\mathbf{k}}(T) - B_{\mathbf{k}}(T)}{2J\sigma E_{\mathbf{k}}(T)}\right]^{\frac{1}{2}} H_{\varepsilon}, \tag{5.4.41b}$$

in the long-wavelength limit. When $\mathbf{k}$ is parallel to the c-axis, (5.4.28) and (5.4.41) predicts that only the transverse phonons with their polarization vectors parallel to the magnetization are coupled to the magnons. The calculation of the velocity of this coupled mode leads, by analogy to (5.4.38), to an elastic constant

$$\frac{c_{44}^*}{c_{44}} = 1 - \frac{\Lambda_{\varepsilon}}{A_{\mathbf{0}}(T) + B_{\mathbf{0}}(T)} \qquad \text{when} \quad \mathbf{f}_{\mathbf{k}}^{\nu} \parallel \langle \mathbf{J} \rangle. \tag{5.4.42}$$

The same result is obtained for the transverse-phonon mode propagating in the direction of the ordered moments, with the polarization vector parallel to the c-axis. These are the two modes which go soft in the case of a second-order transition to a phase with a non-zero c-axis moment.

We have so far only considered the dynamics in the long-wavelength limit. At shorter wavelengths, where the phonon and spin-wave energies may be comparable, the magnon–phonon interaction leads to a strong hybridization of the normal modes, with energy gaps at points in the Brillouin zone where the unperturbed magnon and phonon dispersion relations cross each other, as illustrated in Fig. 5.6. The interaction amplitudes (5.4.28) and (5.4.41b) are correct only for small wave-vectors. At shorter wavelengths, we must consider explicitly the relative positions of neighbouring ions, instead of the local strains. Evenson and Liu (1969) have devised a simple procedure for replacing the local-strain variables in the magnetoelastic Hamiltonian with the relative displacements of the neighbouring ions. Using their procedure, and assuming the nearest-neighbour interactions to be dominant, we find that eqn (5.4.41b) is replaced by

$$W^{\nu}_{\mathbf{k}}(\varepsilon) = -\tfrac{1}{4}c_{\varepsilon}\sqrt{N}\Big(\frac{2}{c}\sin{(kc/2)}\Big)F^{\nu}_{\mathbf{k},\parallel}\left[\frac{A_{\mathbf{k}}(T)-B_{\mathbf{k}}(T)}{2J\sigma E_{\mathbf{k}}(T)}\right]^{\frac{1}{2}}H_{\varepsilon}, \quad (5.4.43)$$

when $\mathbf{k}$ is along the c-axis. c is the lattice constant and $F^{\nu}_{\mathbf{k},\parallel}$ is the component of $\mathbf{F}^{\nu}_{\mathbf{k}}$ parallel to the magnetization vector, which is only non-zero for one of the transverse-phonon modes. This interaction does not distinguish between the two sublattices in the hcp crystal. This means that $W^{\nu}_{\mathbf{k}}(\varepsilon)$ only couples the magnons with the phonons at a certain $\mathbf{k}$ if the modes are either both acoustic or both optical, consistent with the double-zone representation in the c-direction. Except for the replacement of (5.4.41b) by (5.4.43), the interaction Hamiltonian (5.4.41a) is unchanged. From the equations of motion of the Green functions, we may derive the susceptibilities, when $\mathbf{k}$ is along the c-direction, in the same way as before, eqns (5.4.29–36), and the results are found to be:

$$\begin{aligned}\chi_{xx}(\mathbf{k},\omega) &= J\sigma\{A_{\mathbf{k}}(T)-B\mathbf{k}(T)\}\{(\hbar\omega_{t\mathbf{k}})^2-(\hbar\omega)^2\}/\mathcal{D}_{\varepsilon}(\mathbf{k},\omega)\\ \chi_{yy}(\mathbf{k},\omega) &= J\sigma\{A_{\mathbf{k}}(T)+B_{\mathbf{k}}(T)\}\\ &\qquad\times\big\{(\hbar\omega_{t\mathbf{k}})^2-(\hbar\omega)^2-4W^2_{\mathbf{k}}(\varepsilon)\hbar\omega_{t\mathbf{k}}/E_{\mathbf{k}}(T)\big\}/\mathcal{D}_{\varepsilon}(\mathbf{k},\omega),\end{aligned} \quad (5.4.44)$$

with

$$\mathcal{D}_{\varepsilon}(\mathbf{k},\omega) = \{E^2_{\mathbf{k}}(T)-(\hbar\omega)^2\}\{(\hbar\omega_{t\mathbf{k}})^2-(\hbar\omega)^2\}-4W^2_{\mathbf{k}}(\varepsilon)\hbar\omega_{t\mathbf{k}}E_{\mathbf{k}}(T), \quad (5.4.45)$$

where $\omega_{t\mathbf{k}}$ is the angular frequency of the transverse phonon mode at $\mathbf{k}$. Introducing the parameter

$$\Upsilon_{\mathbf{k}} = \left[1+\frac{16\hbar\omega_{t\mathbf{k}}E_{\mathbf{k}}(T)W^2_{\mathbf{k}}(\varepsilon)}{\{E^2_{\mathbf{k}}(T)-(\hbar\omega_{t\mathbf{k}})^2\}^2}\right]^{\frac{1}{2}}, \quad (5.4.46)$$

we find the poles in the susceptibilities at

$$\hbar\omega = \pm E^{\pm}_{\mathbf{k}} = \pm\big[\tfrac{1}{2}\big\{E^2_{\mathbf{k}}(T)+(\hbar\omega_{t\mathbf{k}})^2\big\}\pm\tfrac{1}{2}\big\{E^2_{\mathbf{k}}(T)-(\hbar\omega_{t\mathbf{k}})^2\big\}\Upsilon_{\mathbf{k}}\big]^{\frac{1}{2}}, \quad (5.4.47a)$$

corresponding to

$$\mathcal{D}_{\varepsilon}(\mathbf{k},\omega) = \{(E^{+}_{\mathbf{k}})^2-(\hbar\omega)^2\}\{(E^{-}_{\mathbf{k}})^2-(\hbar\omega)^2\}. \quad (5.4.47b)$$

By a straightforward manipulation of these expressions, we obtain

$$\chi''_{yy}(\mathbf{k},\omega) = \mathrm{Im}\big[\chi_{yy}(\mathbf{k},\omega)\big] = \pi J\sigma \frac{A_{\mathbf{k}}(T)+B_{\mathbf{k}}(T)}{2E_{\mathbf{k}}(T)} \times\Big[\frac{E^+_{\mathbf{k}}}{E_{\mathbf{k}}(T)}\frac{\Upsilon_{\mathbf{k}}+1}{2\Upsilon_{\mathbf{k}}}\big\{\delta(E^+_{\mathbf{k}}-\hbar\omega)-\delta(E^+_{\mathbf{k}}+\hbar\omega)\big\} + \frac{E^-_{\mathbf{k}}}{E_{\mathbf{k}}(T)}\frac{\Upsilon_{\mathbf{k}}-1}{2\Upsilon_{\mathbf{k}}}\big\{\delta(E^-_{\mathbf{k}}-\hbar\omega)-\delta(E^-_{\mathbf{k}}+\hbar\omega)\big\}\Big]. \tag{5.4.48}$$

Almost the same expression is obtained for $\chi''_{xx}(\mathbf{k},\omega)$; the sign before $B_{\mathbf{k}}(T)$ is reversed and the factors $E^{\pm}_{\mathbf{k}}/E_{\mathbf{k}}(T)$ are replaced by their reciprocals. If $W_{\mathbf{k}}(\varepsilon)=0$, then $\Upsilon_{\mathbf{k}}=1$ and $E^+_{\mathbf{k}}=E_{\mathbf{k}}(T)$, and (5.4.48) is equivalent to eqn (5.2.40*b*). When $W_{\mathbf{k}}(\varepsilon)$ is non-zero, $\Upsilon_{\mathbf{k}}>1$ and there are two poles in the magnetic susceptibilities, one at $E^+_{\mathbf{k}}$ closest to $E_{\mathbf{k}}(T)$, and the other at $E^-_{\mathbf{k}}$ closest to the energy of the transverse-phonon mode. Both poles lie outside the energy interval between $E_{\mathbf{k}}(T)$ and $\hbar\omega_{t\mathbf{k}}$. The two normal modes at $\mathbf{k}$, the magnons and the transverse phonons polarized parallel to the magnetization, are transformed into two magnetoelastic modes, both of which give rise to a magnetic scattering of neutrons. The cross-section for neutrons scattered by a pure phonon-mode is proportional to $(\boldsymbol{\kappa}\cdot\mathbf{f}^{\nu}_{\mathbf{k}})^2$. If the scattering vector $\boldsymbol{\kappa}$ is along the *c*-axis, the transverse phonons in this direction do not therefore scatter neutrons, unless they are coupled to the magnons. With $\boldsymbol{\kappa}$ parallel to the *c*-axis, the (magnetic) scattering amplitude is proportional to $\chi''_{yy}(\mathbf{k},\omega)$ and, in this situation, eqn (5.4.48), combined with (4.2.2) and (4.2.3), determines the total scattered intensity due to the coupled magnon and transverse-phonon modes. If the energy difference between the two uncoupled modes at some $\mathbf{k}$ is large, $\Upsilon_{\mathbf{k}}$ is only slightly greater than 1, and the coupling induces only a small repulsion of the mode energies. The pole at energy $E^+_{\mathbf{k}}$, close to the unperturbed magnons, then dominates the magnetic scattering cross-section. The strongest modification occurs at the $\mathbf{k}$-vector where $E_{\mathbf{k}}(T)=\hbar\omega_{t\mathbf{k}}$, at which $\Upsilon_{\mathbf{k}}\to\infty$ and eqn (5.4.48) predicts nearly equal scattering intensities of the two modes at energies determined by

$$(\hbar\omega)^2 = E^2_{\mathbf{k}}(T)\pm 2E_{\mathbf{k}}(T)|W_{\mathbf{k}}(\varepsilon)| \quad ; \quad E_{\mathbf{k}}(T)=\hbar\omega_{t\mathbf{k}}, \tag{5.4.49a}$$

corresponding to an energy splitting, or energy gap, between the two modes of magnitude

$$\Delta \simeq 2|W_{\mathbf{k}}(\varepsilon)|, \tag{5.4.49b}$$

to leading order. These *resonance* or *hybridization* phenomena, the redistribution of the scattered intensity and the creation of an energy gap, are observed whenever two normal modes are coupled linearly with each other, and the value of the energy gap at the **k**-point where the two coupled modes are closest in energy, or where their scattering intensities are equal, gives a direct measure of the coupling amplitude at that particular **k**-vector. The effect of the magnon–phonon interaction on the excitation spectrum in Tb is illustrated in Fig. 5.6.

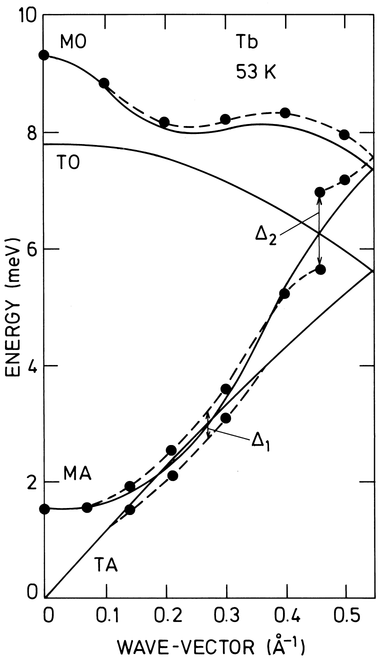

Fig. 5.6. The dispersion relations for the magnons and phonons propagating in the c-direction of Tb at 53 K, illustrating the magnon–phonon interaction. The calculated unperturbed modes are depicted by the full curves. The normal modes are mixed magnon–phonon states, and energy gaps appear at the crossing points of the unperturbed dispersion relations. The acoustic magnons interact both with the acoustic and the optical phonons.

The method described above, based on the magnetoelastic Hamiltonian, is not sufficiently general to enable a prediction of all possible couplings allowed by symmetry, i.e. the *selection rules.* To accomplish this, it is necessary either to use group-theoretical arguments, or to derive a general version of the magnon–phonon Hamiltonian based exclusively on symmetry considerations. These two methods have been applied to this system by respectively Cracknell (1974) and Jensen and Houmann (1975). Their analyses show that, when **k** is along the c-direction, a further mixing is allowed in addition to that considered above. This requires the single-zone representation in the c-direction, since it couples an acoustic mode to an optical mode at the same **k**-vector. The phonon modes in question are once more transverse, but their coupling to the magnons depends on the polarization relative to the direction of magnetization. In an a-axis magnet, the polarization vector should be parallel to the magnetization, as is assumed in eqn (5.4.43), whereas in a b-axis magnet, the acoustic–optical coupling involves the transverse phonons polarized perpendicular to the magnetization (i.e. still along an a-axis). The symmetry arguments show that this coupling must be quadratic in k in the long wavelength limit, instead of linear as is $W_{\mathbf{k}}(\varepsilon)$. It therefore has no influence on the uniform strains or the elastic constants, and accordingly no counterpart in the magnetoelastic Hamiltonian. Liu (1972a) has discussed the possible origin of such an acoustic–optical interaction, and he concludes that it cannot be a crystalline-field effect, but must be mediated indirectly via the conduction electrons and be proportional to the spin–orbit coupling forces. As is illustrated in Fig. 5.6, the acoustic–optical magnon–phonon interaction is clearly observed in Tb, where it leads to the energy gap Δ_2, the strongest hybridization effect seen in the metal. However, a closer examination (Jensen and Houmann 1975) shows that the transverse phonon modes involved are those polarized parallel to the magnetization, in spite of the fact that Tb has its magnetization vector in the b-direction. Hence this interaction violates the selection rules deduced from the general symmetry arguments, leading to the conclusion that the ground-state of Tb cannot be a simple b-axis ferromagnet as assumed. The $4f$ moments are undoubtedly along an easy b-axis, but the spins of the conduction electrons are not necessarily polarized collinearly with the angular momenta of the core electrons, because of their spin–orbit coupling. If the ground-state spin-density wave of the conduction electrons in Tb has a polarization which varies in space within a single unit cell, a coupling mediated by this spin-density wave may violate the selection rules based on the symmetry properties of the simple ferromagnet. The presence of the 'symmetry-breaking' acoustic–optical interaction in Tb demonstrates that the conduction electrons play a more active role than passively transmitting the indirect-exchange interaction. This magnon–phonon coupling is directly dependent on spin–orbit effects in the band electrons, in accordance with Liu's explanation, and its appearance demonstrates that the polarization of the conduction-electron spins must have a component perpendicular to the angular momenta.

To complete this section, we shall briefly discuss the additional magnon–phonon interaction terms which are linear in the phonon operators, but quadratic in the magnon operators:

$$\mathcal{H}_{\mathrm{mp}}^{(2)} = \sum_{\mathbf{qk}\nu} \big[U_\nu(\mathbf{k},\mathbf{q}) \alpha^+_{\mathbf{q}+\mathbf{k}} \alpha_{\mathbf{q}} + \tfrac{1}{2} V_\nu(\mathbf{k},\mathbf{q}) \alpha^+_{\mathbf{q}+\mathbf{k}} \alpha^+_{-\mathbf{q}} + \tfrac{1}{2} V^*_\nu(-\mathbf{k},-\mathbf{q}) \alpha_{\mathbf{q}} \alpha_{-\mathbf{q}-\mathbf{k}} \big] (\beta_{\nu\mathbf{k}} + \beta^+_{\nu-\mathbf{k}}). \quad (5.4.50)$$

Referring back to the magnetoelastic Hamiltonian, we find that such an interaction may originate from, for instance, the term

$$-B_{\gamma 2}\{(O_2^0+O_2^2)-\langle O_2^0+O_2^2\rangle\}\tfrac{1}{2}\cos 2\phi(\epsilon_{\gamma 1}-\overline{\epsilon}_{\gamma 1})$$

in (5.4.6), or the corresponding terms in (5.4.16). In contrast to the linear couplings considered above, the symmetry-preserving α-strain part of the magnetoelastic Hamiltonian makes a contribution to the quadratic interaction terms. Using the procedure of Evenson and Liu (1969), it is straightforward, if somewhat tedious, to relate the interaction amplitudes in eqn (5.4.50) to the magnetoelastic coupling parameters. We shall not perform this analysis here, but refer instead to the detailed calculations of Jensen (1971a,b). The interactions in eqn (5.4.50) have the consequence that the equations of motion of the magnon Green function $\langle\langle \alpha_{\mathbf{q}}\,;\,\alpha^+_{\mathbf{q}}\rangle\rangle$ involve new, higher-order mixed Green functions like $\langle\langle \alpha_{\mathbf{q}-\mathbf{k}}\beta_{\mathbf{k}}\,;\,\alpha^+_{\mathbf{q}}\rangle\rangle$. Performing an RPA or Hartree–Fock decoupling, as in (5.2.29), of the three-operator products which occur in the equations of motion of the new Green functions, we obtain a closed expression for the magnon Green function, which may be written

$$\langle\langle \alpha_{\mathbf{q}}\,;\,\alpha^+_{\mathbf{q}}\rangle\rangle = \frac{1}{\hbar\omega - E_{\mathbf{q}}(T) - \Sigma(\mathbf{q},\omega)}, \tag{5.4.51}$$

where $\Sigma(\mathbf{q},\omega)$ is the *self-energy*, due to the interactions in (5.4.50), of the magnons of wave-vector $\mathbf{q}$. Neglecting $V_\nu(\mathbf{q},\mathbf{k})$, we find that the self-energy at $T=0$ is

$$\Sigma(\mathbf{q},\omega) = \lim_{\epsilon\to 0^+}\sum_{\mathbf{k}\nu}\frac{|U_\nu(\mathbf{k},\mathbf{q})|^2}{\hbar\omega + i\hbar\epsilon - E_{\mathbf{q}+\mathbf{k}}(0) - \hbar\omega_{\nu\mathbf{k}}}\,. \tag{5.4.52}$$

These interactions are not diagonal in reciprocal space and the magnons are therefore affected by all the phonons. Whenever $\mathbf{k}$ has a value such that $E_{\mathbf{q}}(0) \simeq E_{\mathbf{q}+\mathbf{k}}(0) + \hbar\omega_{\nu\mathbf{k}}$, the real part of the denominator in (5.4.52) vanishes close to the magnon pole at $\mathbf{q}$, as determined by (5.4.51). This implies a negative imaginary contribution to $\Sigma(\mathbf{q},\omega)$, when $\hbar\omega \simeq E_{\mathbf{q}}(0)$, and hence a reduction in the lifetime of the magnons. The energy of the magnons at $\mathbf{q}$ is approximately given by $E_{\mathbf{q}}(0) + \mathrm{Re}\big[\Sigma(\mathbf{q},\omega)\big]$, with $\hbar\omega \simeq E_{\mathbf{q}}(0)$. At non-zero temperatures, the self-energy terms increase in proportion to the Bose population-factors of the magnons and phonons involved. These interactions, quadratic in the magnon operators, do not lead to the kind of hybridization effects produced by the linear couplings, but rather give rise to a (small) renormalization of the normal-mode energies and to a finite lifetime of the excitations. These effects are entirely similar to those due to the magnon–magnon interactions appearing in the spin-wave theory in the third order of $1/J$. Equation (5.4.52) shows that the 'zero-point' motion of the ions, at $T = 0$, has a slight effect on the magnons. A similar effect occurs due to the magnon–magnon interactions, but only in an anisotropic ferromagnet where B is non-zero, as we discussed in the previous section. In most cases, the contributions due to the magnon–magnon interactions are expected to predominate, because the magnon–phonon coupling parameters are usually quite small, in comparison with the spin-wave interactions. Although the interactions in (5.4.50) may not be important for the magnons, they may have observable effects on the phonons at finite temperatures. For instance, they affect the velocity of the transverse sound waves propagating in the c-direction and polarized perpendicular to the magnetization, but not those polarized parallel to the magnetization, which are modified by the linear couplings as discussed above. Deriving the perturbed phonon Green functions in the same way as the magnon Green function, and taking the long-wavelength limit, we find (Jensen 1971a,b)

$$\frac{c_{44}^*}{c_{44}} = 1 - \Lambda_\varepsilon \frac{1}{NJ} \sum_{\mathbf{q}} \frac{n_{\mathbf{q}}}{E_{\mathbf{q}}(T)} \qquad \text{when} \quad \mathbf{f}_{\mathbf{k}}^{\nu} \perp \langle \mathbf{J} \rangle. \tag{5.4.53}$$

We note that this result is of higher order in $1/J$ than the effect due to the linear coupling, given in (5.4.42). However, the extra factor $1/J$ may be compensated by the magnon population-factor $n_{\mathbf{q}}$ in the sum over $\mathbf{q}$, at elevated temperatures.

Modifications of the results obtained above may occur, due to anharmonic terms of third order in the strains, or magnetoelastic terms quadratic in the strains. These higher-order contributions may possibly be of some importance for the temperature dependence of the elastic constants and the spin-wave parameters. However, they should be of minor significance under the nearly constant-strain conditions which obtain, for instance, when the magnetic-field dependence of the elastic constants is considered.