5.3 The uniform mode and spin-wave theory

The spin-wave mode at zero wave-vector is of particular interest. In comparison with the Heisenberg ferromagnet, the non-zero energy of this mode is the most distinct feature in the excitation spectrum of the anisotropic ferromagnet. In addition, the magnitude of the energy gap at $\mathbf{q} = \mathbf{0}$ is closely related to the bulk magnetic properties, which may be measured by conventional techniques. We shall first explore the connection between the static magnetic susceptibility and the energy of the uniform mode, leading to an expression for the temperature dependence of the energy gap. In the light of this discussion, we will then consider the general question of the validity of the spin-wave theory which we have presented in this chapter.

5.3.1 The magnetic susceptibility and the energy gap

The static-susceptibility components of the bulk crystal may be determined as the second derivatives of the free energy

$$F = U - TS = -\frac{1}{\beta} \ln Z. \qquad (5.3.1)$$

The specific heat C may be derived in a simple way, within our current spin-wave approximation, by noting that the excitation spectrum is the same as that for a non-interacting Bose system, so that the entropy is fully determined by the statistics of independent bosons of energies $E_{\mathbf{q}}(T)$:

$$S = k_B \sum_{\mathbf{q}} \big[(1+n_{\mathbf{q}})\ln(1+n_{\mathbf{q}}) - n_{\mathbf{q}} \ln n_{\mathbf{q}}\big], \tag{5.3.2}$$

and hence

$$C = T\partial S/\partial T = k_B T \sum_{\mathbf{q}} (dn_{\mathbf{q}}/dT)\ln\{(1+n_{\mathbf{q}})/n_{\mathbf{q}}\},$$

or, with $n_{\mathbf{q}} = \big[e^{\beta E_{\mathbf{q}}(T)} - 1\big]^{-1}$,

$$\begin{aligned} C &= \sum_{\mathbf{q}} E_{\mathbf{q}}(T)\, dn_{\mathbf{q}}/dT \\ &= \beta \sum_{\mathbf{q}} n_{\mathbf{q}}(1+n_{\mathbf{q}})E_{\mathbf{q}}(T)\big\{E_{\mathbf{q}}(T)/T - \partial E_{\mathbf{q}}(T)/\partial T\big\}, \end{aligned} \tag{5.3.3}$$

as in (3.4.17).

The first derivative of F with respect to the angles θ and ϕ can be obtained in two ways. The first is to introduce S, as given by (5.3.2) into (5.3.1), so that

$$\begin{aligned} \frac{\partial F}{\partial \theta} &= \frac{\partial U}{\partial \theta} - \sum_{\mathbf{q}} E_{\mathbf{q}}(T)\frac{\partial n_{\mathbf{q}}}{\partial \theta} \\ &= \frac{\partial U}{\partial \theta}\bigg|_{m_{\mathbf{q}},b_{\mathbf{q}}} + \sum_{\mathbf{q}} \left(\frac{\partial U}{\partial m_{\mathbf{q}}}\frac{\partial m_{\mathbf{q}}}{\partial \theta} + \frac{\partial U}{\partial b_{\mathbf{q}}}\frac{\partial b_{\mathbf{q}}}{\partial \theta} - E_{\mathbf{q}}(T)\frac{\partial n_{\mathbf{q}}}{\partial \theta}\right) \\ &= \frac{\partial U}{\partial \theta}\bigg|_{m_{\mathbf{q}},b_{\mathbf{q}}}, \end{aligned} \tag{5.3.4}$$

as it can be shown that $\partial U/\partial m_{\mathbf{q}} = J\widetilde{A}_{\mathbf{q}}(T)$ and $\partial U/\partial b_{\mathbf{q}} = J\widetilde{B}_{\mathbf{q}}(T)$, when $U = \langle \mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_2 \rangle$, and hence that each term in the sum over $\mathbf{q}$ in the second line of (5.3.4) vanishes, when (5.2.32) is used. This result is only valid to second order in $1/J$. However, a result of general validity is

$$\partial F/\partial \theta = \big\langle \partial \mathcal{H}/\partial \theta \big\rangle, \tag{5.3.5}$$

as discussed in Section 2.1, in connection with eqn (2.1.5). The two different expressions for $\partial F/\partial \theta$, and corresponding expressions for $\partial F/\partial \phi$, agree if $\mathcal{H}$ in (5.3.5) is approximated by $\mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_2$, i.e. to second order in $1/J$. However, the results obtained up to now are based on the additional assumption, which we have not stated explicitly, that $\mathcal{H}'$ in the starting Hamiltonian (5.2.12) is negligible. $\mathcal{H}'$ is the sum of the terms proportional to Stevens operators O_l^m with m odd, and it includes for instance the term $3B_2^0(J_zJ_x+J_xJ_z)\cos\theta\sin\theta$ associated with $B_2^0Q_2^0$ in eqn (5.2.3). $\mathcal{H}'$ vanishes by symmetry if the magnetization is along a high-symmetry direction, i.e. $\theta = 0$ or $\pi/2$ and ϕ is a multiple of $\pi/6$. In these cases, the results obtained previously are valid. If the magnetization is not along a high-symmetry direction, $\mathcal{H}'$ must be taken into account. The first-order contributions arise from terms proportional to $(1/J)^{1/2}$ in $\mathcal{H}'$, which can be expressed effectively as a linear combination of J_x and J_y. In this order, $\langle\partial\mathcal{H}'/\partial\theta\rangle = 0$ therefore, because $\langle J_x\rangle = \langle J_y\rangle = 0$ by definition. For a harmonic oscillator, corresponding in this system to the first order in $1/J$, the condition for the elimination of terms in the Hamiltonian linear in a and a^+ coincides with the equilibrium condition $\partial F/\partial\theta = \partial F/\partial\phi = 0$. Although the linear terms due to $\mathcal{H}'$ can be removed from the Hamiltonian by a suitable transformation, terms cubic in the Bose operators remain. Second-order perturbation theory shows that, if $\mathcal{H}'$ is non-zero, $\langle\partial\mathcal{H}'/\partial\theta\rangle$ and the excitation energies include contributions of the order $1/J^2$. Although it is straightforward to see that $\mathcal{H}'$ makes contributions of the order $1/J^2$, it is not trivial to calculate them. The effects of $\mathcal{H}'$ have not been discussed in this context in the literature, but we refer to the recent papers of Rastelli *et al.* (1985, 1986), in which they analyse the equivalent problem in the case of a helically ordered system.

In order to prevent $\mathcal{H}'$ from influencing the $1/J^2$-contributions derived above, we may restrict our discussion to cases where the magnetization is along high-symmetry directions. This does not, however, guarantee that $\mathcal{H}'$ is unimportant in, for instance, the second derivatives of F. In fact $\partial\langle\partial\mathcal{H}'/\partial\theta\rangle/\partial\theta \propto \mathcal{O}(1/J^2)$ may also be non-zero when $\theta = 0$ or $\pi/2$, and using (5.3.4) we may write

$$\begin{aligned} F_{\theta\theta} &= \frac{\partial^2 F}{\partial\theta^2} = \frac{\partial^2 U}{\partial\theta^2}\bigg|_{m_{\mathbf{q}},b_{\mathbf{q}}} + \mathcal{O}(1/J^2) \\ &= \Big\langle\frac{\partial^2}{\partial\theta^2}(\mathcal{H}_0+\mathcal{H}_1+\mathcal{H}_2)\Big\rangle + \mathcal{O}(1/J^2) \qquad ; \quad \theta = 0,\ \frac{\pi}{2}, \end{aligned} \tag{5.3.6a}$$

and similarly

$$F_{\phi\phi} = \Big\langle\frac{\partial^2}{\partial\phi^2}(\mathcal{H}_0+\mathcal{H}_1+\mathcal{H}_2)\Big\rangle + \mathcal{O}(1/J^2) \qquad ; \quad \phi = p\,\frac{\pi}{6}, \tag{5.3.6b}$$

where the corrections of order $1/J^2$ are exclusively due to $\mathcal{H}'$. Here we have utilized the condition that the first derivatives of $m_{\mathbf{q}}$ and $b_{\mathbf{q}}$ vanish when the magnetization is along a symmetry direction.

The derivatives $F_{\theta\theta}$ and $F_{\phi\phi}$ are directly related to the static susceptibilities, as shown in Section 2.2.2. When $\theta_0 = \frac{\pi}{2}$, we obtain from eqn (2.2.18)

$$\chi_{xx}(\mathbf{0},0) = N\langle J_z\rangle^2/F_{\theta\theta} \quad ; \quad \chi_{yy}(\mathbf{0},0) = N\langle J_z\rangle^2/F_{\phi\phi}. \tag{5.3.7}$$

These results are of general validity, but we shall proceed one step further and use $F(\theta,\phi)$ for estimating the frequency dependence of the bulk susceptibilities. When considering the uniform behaviour of the system, we may to a good approximation assume that the equations of motion for all the different moments are the same:

$$\hbar\partial\langle\mathbf{J}\rangle/\partial t = \langle\mathbf{J}\rangle \times \mathbf{h}(\text{eff}). \tag{5.3.8}$$

By equating it to the average field, we may determine the effective field from

$$F = F(0) - N\langle\mathbf{J}\rangle\cdot\mathbf{h}(\text{eff}), \tag{5.3.9a}$$

corresponding to N isolated moments placed in the field $\mathbf{h}(\text{eff})$. The free energy is

$$F = F(\theta_0,\phi_0) + \tfrac{1}{2}F_{\theta\theta}(\delta\theta)^2 + \tfrac{1}{2}F_{\phi\phi}(\delta\phi)^2 - N\langle\mathbf{J}\rangle\cdot\mathbf{h}, \tag{5.3.9b}$$

and, to leading order, $\delta\theta = -\langle J_x\rangle/\langle J_z\rangle$ and $\delta\phi = -\langle J_y\rangle/\langle J_z\rangle$. Hence

$$h_x(\text{eff}) = -\frac{1}{N}\frac{\partial F}{\partial\langle J_x\rangle} = h_x - \frac{1}{N}F_{\theta\theta}\frac{\langle J_x\rangle}{\langle J_z\rangle^2}, \tag{5.3.10a}$$

and similarly

$$h_y(\text{eff}) = h_y - \frac{1}{N}F_{\phi\phi}\frac{\langle J_y\rangle}{\langle J_z\rangle^2}. \tag{5.3.10b}$$

Introducing a harmonic field applied perpendicular to the z-axis into eqn (5.3.8), we have

$$\begin{aligned} i\hbar\omega\langle J_x\rangle &= \frac{1}{N\langle J_z\rangle}F_{\phi\phi}\langle J_y\rangle - h_y\langle J_z\rangle \\ i\hbar\omega\langle J_y\rangle &= -\frac{1}{N\langle J_z\rangle}F_{\theta\theta}\langle J_x\rangle - h_x\langle J_z\rangle, \end{aligned} \tag{5.3.11}$$

and $\partial\langle J_z\rangle/\partial t = 0$, to leading order in $\mathbf{h}$. Solving the two equations for $h_x = 0$, we find

$$\chi_{yy}(\mathbf{0},\omega) = \langle J_y\rangle/h_y = \frac{1}{N}\frac{F_{\theta\theta}}{E_{\mathbf{0}}^2(T) - (\hbar\omega)^2}, \tag{5.3.12a}$$

and, when $h_y = 0$,

$$\chi_{xx}(\mathbf{0},\omega) = \frac{1}{N}\frac{F_{\phi\phi}}{E_{\mathbf{0}}^2(T) - (\hbar\omega)^2}, \tag{5.3.12b}$$

where the uniform-mode energy is

$$E_{\mathbf{0}}(T) = \frac{1}{N\langle J_z\rangle}\left\{F_{\theta\theta}F_{\phi\phi}\right\}^{1/2}. \tag{5.3.13}$$

This result for the uniform mode in an anisotropic ferromagnet was derived by Smit and Beljers (1955). It may be generalized to an arbitrary magnetization direction by defining (θ,ϕ) to be in a coordinate system in which the polar axis is *perpendicular* to the z-axis (as is the case here), and by replacing $F_{\theta\theta}F_{\phi\phi}$ by $F_{\theta\theta}F_{\phi\phi} - F_{\theta\phi}^2$ if $F_{\theta\phi} \neq 0$.

The introduction of the averaged effective-field in (5.3.8) corresponds to the procedure adopted in the RPA, and a comparison of the results (5.3.12–13) with the RPA result (5.2.40), at $\mathbf{q} = \mathbf{0}$ and $\omega = 0$, shows that the relations

$$\begin{aligned} A_{\mathbf{0}}(T) - B_{\mathbf{0}}(T) &= \frac{1}{N\langle J_z\rangle}F_{\phi\phi} \\ A_{\mathbf{0}}(T) + B_{\mathbf{0}}(T) &= \frac{1}{N\langle J_z\rangle}F_{\theta\theta} \end{aligned} \tag{5.3.14}$$

must be valid to second order in $1/J$. In this approximation, $A_{\mathbf{0}}(T) \pm B_{\mathbf{0}}(T)$ are directly determined by that part of the time-averaged two-dimensional potential, experienced by the single moments, which is quadratic in the components of the moments perpendicular to the magnetization axis. The excitation energy of the uniform mode is thus proportional to the geometric mean of the two force constants characterizing the parabolic part of this potential. Since $A_{\mathbf{0}}(T) \pm B_{\mathbf{0}}(T)$ are parameters of order $1/J$, the second-order contributions of $\mathcal{H}'$ in (5.3.6), which are not known, appear only in order $1/J^3$ in (5.3.14), when the magnetization is along a high-symmetry direction.

B_2^0 does not appear in $A_{\mathbf{0}}(T) - B_{\mathbf{0}}(T)$, and this is in accordance with eqn (5.3.14), as Q_2^0 is independent of ϕ. Considering instead the θ-dependence, we find that the contribution to $F_{\theta\theta}$ is determined by

$$\begin{aligned} \Big\langle \frac{\partial^2 Q_2^0}{\partial\theta^2} \Big\rangle &= \Big\langle -6(J_z^2 - J_x^2)\cos 2\theta - 6(J_zJ_x + J_xJ_z)\sin 2\theta \Big\rangle_{\theta=\pi/2} \\ &= 3\langle O_2^0 - O_2^2\rangle. \end{aligned} \tag{5.3.15}$$

From (5.2.10) and (5.2.11), the thermal average is found to be

$$\begin{aligned} \langle O_2^0 - O_2^2\rangle = 2J^{(2)}\Big\langle 1 - \frac{3}{J}a^+a + \frac{3}{2J^2}a^+a^+aa \\ - \frac{1}{2J}(1 + \tfrac{1}{4J})(aa + a^+a^+) + \frac{1}{4J^2}(a^+aaa + a^+a^+a^+a)\Big\rangle, \end{aligned}$$

or

$$\langle O_2^0 - O_2^2\rangle = 2J^{(2)}\{1 - 3m + 3m^2 + \tfrac{3}{2}b^2 - (1 + \tfrac{1}{4J})b + \tfrac{3}{2}mb + \mathcal{O}(1/J^3)\}. \tag{5.3.16}$$

Hence, according to (5.3.6a) and (5.3.14), the B_2^0-term contributes to the spin-wave parameter $A_{\mathbf{0}}(T) + B_{\mathbf{0}}(T)$ by

$$\begin{aligned} 3B_2^0\langle O_2^0 - O_2^2\rangle/\langle J_z\rangle &\simeq 6B_2^0 J^{(2)}(1 - 3m - b)/J(1 - m) \\ &\simeq 6B_2^0 J^{(2)}(1 - 2m - b)/J, \end{aligned}$$

in agreement with (5.2.37b). When b is zero, this result is consistent with the classical Zener power-law (Zener 1954), $\langle O_l^m\rangle \propto \delta_{m0}\,\sigma^{l(l+1)/2}$, where $\sigma = 1 - m$ is the relative magnetization, since, to the order considered, $\langle O_2^0 - O_2^2\rangle_{b=0} = \langle O_2^0\rangle_{b=0} = 2J^{(2)}(1 - m)^3$. If we include the diagonal contribution of third order in m or $1/J$ to $\langle O_2^0\rangle$ in (5.3.16), the result differs from the Zener power-law, but agrees, at low temperatures, with the more accurate theory of Callen and Callen (1960, 1965) discussed in Section 2.2. The results of the linear spin-wave theory obtained above can be utilized for generalizing the theory of Callen and Callen to the case of an anisotropic ferromagnet. The elliptical polarization of the spin waves introduces corrections to the thermal expectation values, which we express in the form

$$\langle O_2^0 - O_2^2\rangle = 2J^{(2)}\hat{I}_{5/2}[\sigma]\,\eta_+^{-1}, \tag{5.3.17}$$

where the factor $\hat{I}_{l+1/2}[\sigma]$ represents the result (2.2.5) of Callen and Callen, and where $\eta_\pm$ differs from 1 if b is non-zero. The two correlation functions m and b are determined through eqn (5.2.32), in terms of the intermediate parameters $\widetilde{A}_{\mathbf{k}}(T) \pm \widetilde{B}_{\mathbf{k}}(T)$, but it is more appropriate to consider instead

$$\begin{aligned} m_o &= \frac{1}{NJ}\sum_{\mathbf{k}}\Big\{\frac{A_{\mathbf{k}}(T)}{E_{\mathbf{k}}(T)}\big(n_{\mathbf{k}} + \tfrac{1}{2}\big) - \tfrac{1}{2}\Big\} \\ b_o &= -\frac{1}{NJ}\sum_{\mathbf{k}}\frac{B_{\mathbf{k}}(T)}{E_{\mathbf{k}}(T)}\big(n_{\mathbf{k}} + \tfrac{1}{2}\big), \end{aligned} \tag{5.3.18}$$

defined in terms of the more fundamental parameters. The transformation (5.2.34) then leads to the following relations:

$$m_o + \tfrac{1}{2J} = m + \tfrac{1}{2J} - \tfrac{1}{2}b^2 \qquad \text{and} \quad b_o = b - \tfrac{1}{2}b(m + \tfrac{1}{2J}).$$

Separating the two contributions in (5.3.16), we find

$$\widetilde{b} \equiv \langle O_2^2\rangle/\langle O_2^0\rangle \simeq (1 + \tfrac{1}{4J})b(1 - m)^{-3/2}, \tag{5.3.19a}$$

which, to the order calculated, may be written

$$\widetilde{b} = \big(1 - \frac{1}{2J}\big)^{-1} \frac{b_o}{\sigma^2}, \tag{5.3.19b}$$

where

$$\sigma = \langle J_z \rangle / J = 1 - m = 1 - m_o - \tfrac{1}{2} b_o \widetilde{b}. \tag{5.3.20}$$

The function $\eta_\pm$ is then determined in terms of $\widetilde{b}$ as

$$\eta_\pm = (1 \pm \widetilde{b})(1 - \tfrac{1}{2}\widetilde{b}^2). \tag{5.3.21}$$

The spin-wave theory determines the correlation functions σ and $\eta_\pm$ to second order in $1/J$, but for later convenience we have included some higher-order terms in (5.3.20) and (5.3.21). It may be straightforwardly verified that the thermal expectation values of $\langle O_2^0 - O_2^2 \rangle$ given by (5.3.16) and (5.3.17) agree with each other to order $1/J^2$. In the absence of anisotropy, the latter has a wider temperature range of validity than the former, extending beyond the regime where the excitations can be considered to be bosons. This should still be true in the presence of anisotropy, as long as $\widetilde{b}$ is small.

The combination of the spin-wave theory and the theory of Callen and Callen has thus led to an improved determination of the thermal averages of single-ion Stevens operators, as shown in Figs. 2.2 and 2.3. The quantity $O_2^0 - O_2^2$ was chosen as an example, but the procedure is the same for any other single-ion average. It is tempting also to utilize this improvement in the calculation of the excitation energies, and the relation (5.3.14) between the free energy and the spin-wave parameters $A_{\mathbf{0}}(T) \pm B_{\mathbf{0}}(T)$ is useful for this purpose. Neglecting the modifications due to $\mathcal{H}'$ in (5.3.6), i.e. using $F_{\theta\theta} \simeq \langle \partial^2 \mathcal{H} / \partial \theta^2 \rangle$ and similarly for $F_{\phi\phi}$, we find from (5.3.14) the following results:

$$A_{\mathbf{0}}(T) - B_{\mathbf{0}}(T) = -\frac{1}{J\sigma} 36 B_6^6 J^{(6)} \hat{I}_{13/2}[\sigma] \eta_-^{-15} \cos 6\phi + g\mu_B H \cos(\phi - \phi_H) \tag{5.3.22a}$$

and

$$\begin{aligned} A_{\mathbf{0}}(T) + B_{\mathbf{0}}(T) = \frac{1}{J\sigma} \Big[& 6 B_2^0 J^{(2)} \hat{I}_{5/2}[\sigma] \eta_+^{-1} - 60 B_4^0 J^{(4)} \hat{I}_{9/2}[\sigma] \eta_-^7 \eta_+^{-1} \\ & + 210 B_6^0 J^{(6)} \hat{I}_{13/2}[\sigma] \eta_-^{18} \eta_+^{-1} - 6 B_6^6 J^{(6)} \hat{I}_{13/2}[\sigma] \eta_-^{-30} \eta_+^{-25} \cos 6\phi \Big] \\ & + g\mu_B H \cos(\phi - \phi_H), \end{aligned} \tag{5.3.22b}$$

which for completeness include all contributions from the starting Hamiltonian (5.2.1). The spin-wave spectrum at non-zero wave-vectors is adjusted accordingly by inserting $A_{\mathbf{0}}(T) \pm B_{\mathbf{0}}(T)$ given above, instead of (5.2.37), in eqns (5.2.36), (5.2.38), and (5.2.40). If the out-of-plane anisotropy is stronger than the in-plane anisotropy, as in Tb and Dy, B is positive and $\widetilde{b}$ is negative. This means that η_+ and η_- are respectively smaller and greater than 1 (for small $\widetilde{b}$), with the result that the axial contributions to $A_{\mathbf{0}}(T) + B_{\mathbf{0}}(T)$ are increased, whereas the planar contribution to $A_{\mathbf{0}}(T) - B_{\mathbf{0}}(T)$ is diminished, due to $\widetilde{b}$. This is consistent with the fact that the out-of-plane fluctuations are suppressed in comparison with the in-plane fluctuations by the anisotropy. Hence we find, as a general result, that the elliptical polarization of the spin waves enhances, in a self-consistent fashion, the effects of the anisotropy. We note that Q_6^6, which depends on both θ and ϕ, contributes to both anisotropy parameters, but that the anisotropy of the fluctuations affects the two contributions differently.

If $\widetilde{b}$ and the **k**-sums in (5.2.38) are neglected, the above result for the spin-wave energies $E_{\mathbf{q}}(T)$ reduces to that derived by Cooper (1968b). The modifications due to the non-spherical precession of the moments, $\widetilde{b} \neq 0$, were considered first by Brooks *et al.* (1968) and Brooks (1970), followed by the more systematic and comprehensive analysis of Brooks and Egami (1973). They utilized directly the equations of motion of the angular-momentum operators, without introducing a Bose representation. Their results are consistent with those above, except that they did not include all the second-order modifications considered here. We also refer to Tsuru (1986), who has more recently obtained a result corresponding to eqn (5.2.31), when B_6^6 is neglected, using a variational approach. The procedure outlined above essentially follows that of Lindgård and Danielsen (1974, 1975), which was further developed by Jensen (1975). This account only differs from that given by Jensen in the use of $\eta_\pm$ instead of $\widetilde{b}$ as the basis for the 'power-law' generalization (and by the alternative choice of sign for B and $\widetilde{b}$) and, more importantly, by the explicit use of $1/J$ as the expansion parameter.

As illustrated in Fig. 5.1 for Gd, and in Fig. 5.3 for Tb, the observed temperature dependence of the spin-wave spectrum is indeed substantial, both in the isotropic and the anisotropic ferromagnet. In the case of Tb, the variation of the exchange contribution is augmented by the temperature dependence of the anisotropy terms, which is reflected predominantly in the rapid variation of the energy gap at $\mathbf{q} = \mathbf{0}$. A comparison of Figs. 5.1 and 5.3 shows that the change in the form of $\mathcal{J}(\mathbf{q})$ appears to be more pronounced in Tb than in Gd. In Tb, the variation of $\mathcal{J}(\mathbf{q})$ with $\mathbf{q}$ at a particular temperature is also modified if the magnetization vector is rotated from the b-axis to a hard a-axis (Jensen *et al.* 1975). Most of these changes with magnetization can be explained as the result of two-ion anisotropy, which we will consider in Section 5.5. Anisotropic two-ion terms may also affect the energy gap. In addition,

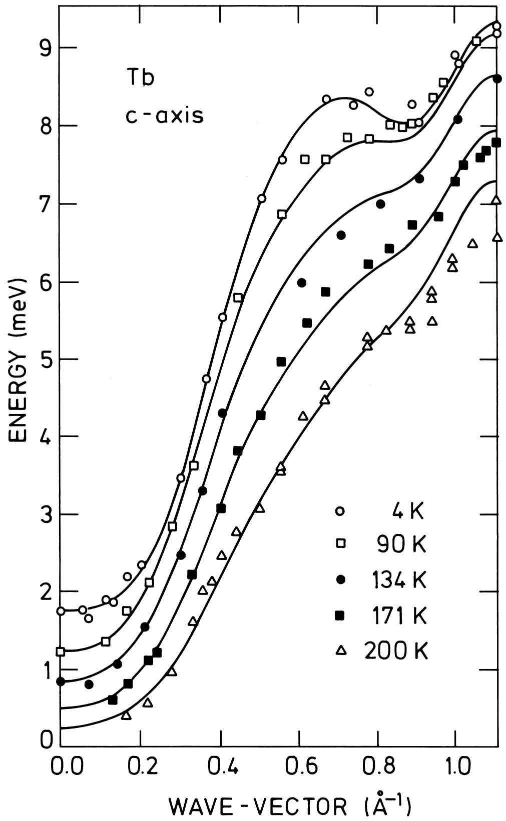

Fig. 5.3. The temperature dependence of the dispersion relations for the unperturbed spin waves in the c-direction in Tb. Both the energy gap and the **q**-dependence renormalize with temperature. The results have been corrected for the magnon–phonon interaction, and the lines show the calculated energies.

the magnetoelastic coupling introduces qualitatively new effects, not describable by eqn (5.3.22), to which we will return after a short digression to summarize our understanding of the spin-wave theory.

5.3.2 The validity of the spin-wave theory

In presenting the spin-wave theory, we have neglected phenomena which first appear in the third order of $1/J$, most importantly the finite lifetimes of the excitations. In the presence of anisotropy, when B is different from zero, the total moment is not a conserved quantity, since $[\sum_i J_{iz}\, , \mathcal{H}] \neq 0$, unlike in the Heisenberg model. On the microscopic plane, this means that the number of spin-wave excitations, i.e. magnons, is not necessarily conserved in a scattering process. In contrast to the behaviour of the isotropic ferromagnet, the linewidths do not therefore vanish at zero temperature, although energy conservation, combined with the presence of an energy gap in the magnon spectrum, strongly limit the importance of the allowed decay processes at low temperatures.

The two-ion interactions are assumed to involve only tensor operators of the lowest rank, so that these terms in the $1/J$-expansion only have small numerical factors multiplying the Bose operator products. Therefore, if J is large, as in heavy rare earth-ions, the third-order terms due to the exchange coupling, which are neglected in the spin-wave theory, are expected to be small, as long as the number of excited magnons is not very large. The weak influence, at low temperatures, of the higher-order contributions of the exchange coupling is also indicated by a comparison with the low-temperature expansion of Dyson (1956) of the free energy in a Heisenberg ferromagnet with only nearest-neighbour interactions, also discussed by Rastelli and Lindgård (1979). If $A = B = 0$, the results derived earlier, to second order in $1/J$, are consistent with those of Dyson, except that we have only included the leading-order contribution, in the Born approximation or in powers of $1/J$, to the T^4-term in the magnetization and in the specific heat. The higher-order corrections to the T^4-term are significant if $J = \frac{1}{2}$, but if $J = 6$ as in Tb, for example, they only amount to a few per cent of this term and can be neglected.

If only the two-ion terms are considered, the RPA decoupling of the Bose operator products (5.2.29) is a good approximation at large J and at low temperatures. However, this decoupling also involves an approximation to the single-ion terms, and these introduce qualitatively new features into the spin-wave theory in the third order of $1/J$. For example, the C_3-term in (5.2.26) directly couples the $|J_z = J>$ state and $|J-4>$, leading to an extra modification of the ground state not describable in terms of B or $\eta_\pm$. Furthermore, the Bogoliubov transformation causes the (J_x, J_y)-matrix elements between the ground state and the third excited state to become non-zero. This coupling then leads to the appearance of a new pole in the transverse susceptibilities, in addition to the spin-wave pole, at an energy which, to leading order, is roughly independent of $\mathbf{q}$ and close to that of the third excited MF level, i.e. $3E_{\mathbf{q}_o}(T)$, with $\mathbf{q}_o$ defined as a wave-vector at which $\mathcal{J}(\mathbf{q}_o) = 0$. A qualitative analysis indicates that the third-order contribution to e.g. $\chi_{xx}(\mathbf{0}, 0)$, due to this pole, must cancel the second-order contribution of $\mathcal{H}'$ to $F_{\theta\theta}$ in the relation (5.3.12b) between the two quantities. Hence the approximation $F_{\theta\theta} \simeq \langle \partial^2 \mathcal{H}/\partial\theta^2 \rangle$, used in (5.3.22), corresponds to the neglect of this additional pole.

The higher-order exchange contributions can thus be neglected at low temperatures, if J is large. This condition is not, however, sufficient to guarantee that the additional MF pole is unimportant, and the spin-wave result (5.3.22), combined with (5.2.36), (5.2.38), and (5.2.40), can only be trusted as long as the modification of the ground state, due to the single-ion anisotropy, is weak. This condition is equivalent to the requirement that $|\widetilde{b}|$ be much less than 1. The regime within which the spin-wave theory is valid can be examined more closely by a comparison with the MF-RPA theory. In the latter, only the two-ion interactions are treated approximately, whereas the MF Hamiltonian is diagonalized exactly. The MF-RPA decoupling utilized in Section 3.5 leads here to a cancellation of the $\mathbf{k}$-sums in (5.3.38), and to a replacement of the correlation functions m_o and b_o by their MF values

$$m_o \simeq m_o^{\mathrm{MF}} = \frac{1}{J}\left\{\frac{A_{\mathbf{q}_o}(T)}{E_{\mathbf{q}_o}(T)}\big(n_{\mathbf{q}_o} + \tfrac{1}{2}\big) - \tfrac{1}{2}\right\}, \tag{5.3.23}$$

with a similar expression for b_o^{MF}. The wave-vector $\mathbf{q}_o$ is defined as above, such that $\mathcal{J}(\mathbf{q}_o) = 0$. If the single-ion anisotropy is of second rank only, including possibly a Q_2^2-term as well as the Q_2^0-term of our specific model, all the predictions obtained with the MF-RPA version of the spin-wave theory agree extremely well with the numerical results obtained by diagonalizing the MF Hamiltonian exactly, even for relatively large values of $|b_o^{\mathrm{MF}}|$ (≈ 0.1). Even though $1/J$ is the expansion parameter, the replacement of $(1+\frac{1}{2J})$ by $(1-\frac{1}{2J})^{-1}$ in (5.3.19b) extends the good agreement to the limit $J = 1$, in which case the MF Hamiltonian can be diagonalized analytically.

The applicability of the $1/J$-expansion for the anisotropy is much more restricted if terms of high rank, such as Q_6^6, dominate. This is a simple consequence of the relatively greater importance of the contributions of higher-order in $1/J$, like for instance the C_3-term in (5.2.26), for higher-rank anisotropy terms. We have analysed numerically models corresponding to the low-temperature phases of Tb and Er, which include various combinations of anisotropy terms with ranks between 2 and 6. In the case of the basal-plane ferromagnet Tb, we find that the $1/J$-expansion leads to an accurate description of the crystal-field effects on both the ground-state properties and the excitation energies. The MF-RPA excitation-energies calculated with the procedure of Section 3.5 differ relatively only by $\sim 10^{-3}$ at $T = 0$ from those of the spin-wave theory (Jensen 1976c). We furthermore find that this good agreement extends to non-zero temperatures, and that the $1/J$-expansion is still acceptably accurate when $\sigma \simeq 0.8$. Consequently, the effective power-laws predicted by the spin-wave theory at low temperatures (Jensen 1975) are valid.

The renormalization of the anisotropy parameters appearing in the spin-wave energies, in the second order of $1/J$, is expected to be somewhat more important in the conical phase of Er than in Tb. In Er, the moments are not along a symmetry direction (they make an angle of about 28° with the c-axis) and the second-order modifications due to $\mathcal{H}'$ in (5.2.12) might be expected to be important. The $1/J$-results do not allow a precise estimate of the second-order contributions, but by introducing two scaling parameters, one multiplying the exchange terms by σ, and the other scaling the constant crystal-field contribution in the $1/J$-expression for the spin-wave energies in the cone phase, it is possible (Jensen 1976c) to give an accurate account of the excitation energies derived by diagonalizing the MF Hamiltonian exactly, the relative differences being only of the order 10^{-2}. The two scaling parameters are found to have the expected magnitudes, although σ turns out to be slightly smaller ($\simeq 0.94$ in the model considered) than the relative magnetization predicted by the MF Hamiltonian ($\sigma^{\rm MF} \simeq 0.98$). An analysis of the MF Hamiltonian shows that the excitations can be described in terms of an elliptical precession of the single moments, as expected, but surprisingly the ellipsoid lies in a plane with its normal making an angle ($\simeq 33°$) with the c-axis which differs from the equilibrium cone-angle ($\simeq 28°$), so the polarization of the spin waves is not purely transverse. In terms of the $1/J$-expansion, this modification of the excited states can only be produced by $\mathcal{H}'$. This observation indicates that $\mathcal{H}'$ has significant effects in Er, since it explains the difference between σ and $\sigma^{\rm MF}$, as σ becomes equal to $\sigma^{\rm MF}$ if the angle appearing in the renormalized spin-wave energies is considered to be that defining the excited states, i.e. 33°, rather than the equilibrium value.

We may conclude that the $1/J$-expansion is a valid procedure for describing the low-temperature magnetic properties of the heavy rare earth metals. This is an important conclusion for several reasons. To first order in $1/J$, the theory is simple and transparent. It is therefore feasible to include various kinds of complication in the model calculations and to isolate their consequences. This simplicity is retained in the second order of $1/J$, as long as $\mathcal{H}'$ can be neglected, in which case the first-order parameters are just renormalized. Accurate calculations of the amount of renormalization of the different terms may be quite involved, but because of the long range of the two-ion interactions in the rare earth metals, the MF values of m_o and b_o utilized above normally provide good estimates. The spin-wave theory in the harmonic approximation, to first order in $1/J$, has been employed quite extensively in the literature, both for analysing experimental results and in various theoretical developments. It is therefore fortunate that these analyses are not invalidated, but only modified, or renormalized, by the presence of moderate anisotropy. However, it is necessary to be aware that the renormalization itself may cause special effects not expected in the harmonic approximation, as the amount of renormalization may change when the system is perturbed by an external magnetic field or pressure, or when the temperature is altered.

There have been attempts (Lindgård 1978, and references therein) to construct an analytical spin-wave theory starting with a diagonalization of the MF Hamiltonian. In principle, this should be an appropriate starting-point, since the ground state is closer to the MF ground-state than to the fully polarized state, as soon as the planar anisotropy becomes significant. As in the model calculations discussed above, the MF Hamiltonian can be diagonalized numerically without difficulty, but in this form the method is non-analytical and the results are not easily interpretable. In order to diagonalize the MF Hamiltonian analytically, one is forced to make a perturbative expansion, unless J is small. If the MF Hamiltonian is expressed in the $|J_z>$-basis, the natural expansion parameter is $\sim |B_{\mathbf{q}_o}/A_{\mathbf{q}_o}| \simeq 2J|b_o|$ at $T=0$. The use of this expansion parameter and the $1/J$-expansion considered above lead to identical results in the limit $2J|b_o| \ll 1$ (Rastelli and Lindgård 1979). However, the expansion parameter is not small when the anisotropy is moderately large ($2J|b_o| \simeq 0.35$ in Tb at $T=0$), which severely limits the usefulness of this procedure as applied by Lindgård (1978, 1988) to the analysis of the spin waves in the anisotropic heavy rare earths. It gives rise to a strong renormalization of all the leading-order spin-wave-energy parameters, which are thus quite sensitive, for example, to an external magnetic field, and it is extremely difficult to obtain a reasonable estimate of the degree of renormalization. In contrast, the $1/J$-expansion leads, at low temperatures, to results in which only the high-rank terms (which are quite generally of smaller magnitude than the low-rank terms) are renormalized appreciably, and the amount of renormalization can be determined with fair accuracy. In the numerical example corresponding to Tb, the B_6^6-term is renormalized by -38% at $T=0$, according to the spin-wave theory, which agrees with the value obtained by diagonalizing the MF Hamiltonian exactly, as indicated in Fig. 2.3.

To recapitulate, we have developed a self-consistent RPA theory for the elementary excitations in a ferromagnet, i.e. the spin waves, valid when the magnetization is close to its saturation value. The major complication is the occurrence of anisotropic single-ion interactions, which were treated by performing a systematic expansion in $1/J$. To first order in $1/J$, the theory is transparent and simple, and it is straightforwardly generalized to different physical situations. Much of the simplicity is retained in second order, as long as the magnetization is along a symmetry axis, but the first-order parameters are replaced by effective values. These effective parameters are determined self-consistently in terms of the spin-wave parameters $A_{\mathbf{q}}(T) \pm B_{\mathbf{q}}(T)$, which depend on T, and on an eventual applied magnetic field. One advantage of the use of $1/J$ as the expansion parameter is that the second-order modifications are smallest for the low-rank couplings, which are quite generally also the largest terms. If the magnetization is not along a symmetry axis, the elementary excitations may no longer be purely transverse. This additional second-order phenomenon may, however, be very difficult to detect experimentally within the regime of validity of the second-order spin-wave theory.