

## 5.2 Spin waves in the anisotropic ferromagnet

In the heavy rare earth metals, the two-ion interactions are large and of long range. They induce magnetically-ordered states at relatively high temperatures, and the ionic moments approach closely their saturation values at low temperatures. These circumstances allow us to adopt a somewhat different method, *linear spin-wave theory*, from those discussed previously in connection with the derivation of the correlation functions. We shall consider the specific case of a hexagonal close-packed crystal ordered ferromagnetically, with the moments lying in the basal plane, corresponding to the low-temperature phases of both Tb and Dy. For simplicity, we shall initially treat only the anisotropic effects introduced by the single-ion crystal-field Hamiltonian so that, in the case of hexagonal symmetry, we have

$$\mathcal{H} = \sum_i \left[ \sum_{l=2,4,6} B_l^0 Q_l^0(\mathbf{J}_i) + B_6^6 Q_6^6(\mathbf{J}_i) - g\mu_B \mathbf{J}_i \cdot \mathbf{H} \right] - \frac{1}{2} \sum_{i \neq j} \mathcal{J}(ij) \mathbf{J}_i \cdot \mathbf{J}_j. \quad (5.2.1)$$

The system is assumed to order ferromagnetically at low temperatures, a sufficient condition for which is that the maximum of  $\mathcal{J}(\mathbf{q})$  occurs at  $\mathbf{q} = \mathbf{0}$ .  $Q_l^m(\mathbf{J}_i)$  denotes the Stevens operator of the  $i$ th ion, but defined in terms of  $(J_\xi, J_\eta, J_\zeta)$  instead of  $(J_x, J_y, J_z)$ , where the  $(\xi, \eta, \zeta)$ -axes are fixed to be along the symmetry  $a$ -,  $b$ - and  $c$ -directions, respectively, of the hexagonal lattice. The  $(x, y, z)$ -coordinate system is chosen such that the  $z$ -axis is along the magnetization axis, specified by the polar angles  $(\theta, \phi)$  in the  $(\xi, \eta, \zeta)$ -coordinate system. Choosing the  $y$ -axis to lie in the basal plane, we obtain the following relations:

$$\begin{aligned} J_\xi &= J_z \sin \theta \cos \phi - J_x \cos \theta \cos \phi + J_y \sin \phi \\ J_\eta &= J_z \sin \theta \sin \phi - J_x \cos \theta \sin \phi - J_y \cos \phi \\ J_\zeta &= J_z \cos \theta + J_x \sin \theta, \end{aligned} \quad (5.2.2)$$

from which

$$Q_2^0 = 3\{J_z^2 \cos^2 \theta + J_x^2 \sin^2 \theta + (J_z J_x + J_x J_z) \cos \theta \sin \theta\} - J(J+1). \quad (5.2.3)$$

Initially we assume that  $\langle J_z \rangle = J$  at  $T = 0$ , which implies that the ground state is the product of  $|J_z = J\rangle$ -states of the single ions. In this case, we find, consistently with eqn (2.2.14),

$$\langle Q_2^0 \rangle = \langle J | Q_2^0 | J \rangle = J^{(2)}(3 \cos^2 \theta - 1),$$

where, as before,  $J^{(n)} = J(J - \frac{1}{2}) \cdots (J - \frac{n-1}{2})$ , and we have used the expectation values  $\langle J_z^2 \rangle = J^2$ ,  $\langle J_x^2 \rangle = \frac{1}{2}J$  and  $\langle J_z J_x \rangle = 0$ . Analogously, though with considerably more labour, we can show that, for instance,

$$\langle Q_6^0 \rangle = \langle J | \frac{1}{2}(J_\xi + iJ_\eta)^6 + \frac{1}{2}(J_\xi - iJ_\eta)^6 | J \rangle = J^{(6)} \sin^6 \theta \cos 6\phi. \quad (5.2.4)$$

For simplicity, we neglect for the moment  $B_4^0$  and  $B_6^0$ , and specifying the direction of the magnetic field by the polar angles  $(\theta_H, \phi_H)$ , we find that the ground-state energy is, within this approximation,

$$\begin{aligned} U(T=0) \simeq N [ & B_2^0 J^{(2)}(3 \cos^2 \theta - 1) + B_6^0 J^{(6)} \sin^6 \theta \cos 6\phi \\ & - g\mu_B JH \{ \cos \theta \cos \theta_H + \sin \theta \sin \theta_H \cos(\phi - \phi_H) \} - \frac{1}{2} \mathcal{J}(\mathbf{0}) J^2 ], \end{aligned} \quad (5.2.5)$$

where  $\theta$  and  $\phi$  are determined so that they minimize this expression. In zero magnetic field,  $H = 0$ , (5.2.5) only gives two possibilities for  $\theta$ , viz.  $\theta = 0$  for  $B_2^0 J^{(2)} < -\frac{1}{3}|B_6^0|J^{(6)}$  or  $\theta = \frac{\pi}{2}$  for  $B_2^0 J^{(2)} > -\frac{1}{3}|B_6^0|J^{(6)}$ . We shall here be concerned with the second case of  $\theta = \frac{\pi}{2}$ , i.e. the basal-plane ferromagnet. In this case, the angle  $\phi$  is determined by the sign of  $B_6^0$ . The magnetic moments will be along an  $a$ - or a  $b$ -axis ( $\phi = 0$  or  $\phi = \frac{\pi}{2}$ ) if  $B_6^0$  is respectively negative or positive. Having specified the (approximate) ground state, we turn to the excitations, i.e. the spin waves.

Instead of utilizing the standard-basis operators, defined by (3.5.11), we shall introduce a Bose operator  $a_i$  for the  $i$ th ion, satisfying

$$[a_i, a_j^+] = \delta_{ij} \quad ; \quad [a_i, a_j] = [a_i^+, a_j^+] = 0, \quad (5.2.6)$$

which acts on the  $|J_z\rangle$ -state vector of this ion (the site index is suppressed) in the following way:

$$a |J\rangle = 0 \quad ; \quad a |J - m\rangle = \sqrt{m} |J - m + 1\rangle \quad (5.2.7)$$

Holstein and Primakoff (1940) introduced the following representation of the angular momentum operators:

$$\begin{aligned} J_z &= J - a^+ a \\ J_+ &= (2J - a^+ a)^{\frac{1}{2}} a \\ J_- &= a^+ (2J - a^+ a)^{\frac{1}{2}}. \end{aligned} \quad (5.2.8)$$

If the usual basis vectors in the Hilbert space created by the Bose operators are denoted by  $|n\rangle$ , i.e.  $a|n\rangle = \sqrt{n}|n-1\rangle$  where  $n = 0, 1, 2, \dots, \infty$ , then by the definition (5.2.7),  $|n\rangle = |J_z = J-n\rangle$  for  $n = 0, 1, 2, \dots, 2J$ , but there is no physical  $|J_z\rangle$ -state corresponding to  $|n\rangle$  when  $n > 2J$ . It is straightforward to see that the Bose representation (5.2.8) produces the right matrix-elements of the angular momentum operators, as long as  $|n\rangle$  is restricted to the physical part of the Hilbert space,  $n \leq 2J$ , but this representation presupposes the presence of an infinite number of states. In the ferromagnetic case, the unphysical states are at high energies, if  $J$  is large and  $T$  is low, and their influence on the thermal averages is negligible. In this regime of  $J$  and  $T$ , the *Holstein-Primakoff transformation* is useful and the results derived from it are trustworthy.

In order to be able to treat the Bose operators under the square roots in eqn (5.2.8), we shall utilize  $1/J$  as an expansion parameter. This means that, instead of the  $J_{\pm}$  given by (5.2.8), we shall use

$$J_+ = (J_-)^\dagger \simeq \sqrt{2J} \left( a - \frac{1}{4J} a^+ a a \right). \quad (5.2.9)$$

It is important here to realize that the expansion parameter is  $1/J$  and not, for instance, ‘the number of deviation operators’. If the latter were the case, a well-ordered expansion of  $J_+$  (Lindgård and Danielsen 1974) would suggest instead  $J_+ = \sqrt{2J} \{ a - (1 - \sqrt{1 - 1/2J}) a^+ a a + \dots \}$ , corresponding to a replacement of  $\frac{1}{4J}$  in (5.2.9) by  $\frac{1}{4J} (1 + \frac{1}{8J} + \dots)$ . We emphasize that we shall be expanding the *reduced* operators  $(1/J^{(l)}) O_l^m$ , leaving no ambiguities either in (5.2.9) or in the following. Using eqn (5.2.9) and  $J_z = J - a^+ a$ , it is straightforward to express the Stevens operators in terms of the Bose operators. For  $O_2^0$ , we get

$$\begin{aligned} O_2^0 &= 3J_z^2 - J(J+1) = 3(J - a^+ a)^2 - J(J+1) \\ &= 2J(J - \frac{1}{2}) - 6(J - \frac{1}{2}) a^+ a + 3a^+ a^+ a a \\ &= 2J^{(2)} \left\{ 1 - \frac{3}{J} a^+ a + \frac{3}{2J^2} a^+ a^+ a a + \mathcal{O}(1/J^3) \right\}. \end{aligned} \quad (5.2.10)$$

Here we have used  $[a, a^+] = 1$  to arrange the operators in ‘well-ordered’ products, with all the creation operators to the left, and in the last line  $1/J^{(2)}$  has been replaced by  $1/J^2$  in the term of second order in  $1/J$ . In the same way, we obtain

$$\begin{aligned} O_2^2 &= \frac{1}{2}(J_+^2 + J_-^2) = J^{(2)} \left\{ \frac{1}{J} (a^+ a^+ + a a) \right. \\ &\quad \left. + \frac{1}{4J^2} (a^+ a^+ + a a - 2a^+ a^+ a^+ a - 2a^+ a a a) + \mathcal{O}(1/J^3) \right\}. \end{aligned} \quad (5.2.11)$$

The expression for  $Q_2^0$  is then determined using  $Q_2^0(\theta = \frac{\pi}{2}) = -\frac{1}{2}O_2^0 + \frac{3}{2}O_2^2$ . For the case of  $Q_6^6$ , we refer to Lindgård and Danielsen (1974), who have established the Bose operator expansion of the tensor operators up to the eighth rank. Introducing these expansions into (5.2.1), and grouping the terms together according to their order in  $1/J$ , we may write the Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_2 + \cdots + \mathcal{H}', \quad (5.2.12)$$

where  $\mathcal{H}_0 = U_0$  is the zero-order term, and

$$U_0 = N \left[ -B_2^0 J^{(2)} + B_6^6 J^{(6)} \cos 6\phi - g\mu_B JH \cos(\phi - \phi_H) - \frac{1}{2} J^2 \mathcal{J}(\mathbf{0}) \right], \quad (5.2.13)$$

corresponding to (5.2.5), when we restrict ourselves to the case  $\theta = \theta_H = \pi/2$ .  $\mathcal{H}_1$  comprises the terms of first order in  $1/J$ , and is found to be

$$\mathcal{H}_1 = \sum_i \left[ A a_i^+ a_i + B \frac{1}{2} (a_i^+ a_i^+ + a_i a_i) \right] - \sum_{ij} J \mathcal{J}(ij) (a_i^+ a_j - a_i^+ a_i), \quad (5.2.14)$$

where the parameters  $A$  and  $B$  are

$$\begin{aligned} A &= \frac{1}{J} \{ 3B_2^0 J^{(2)} - 21B_6^6 J^{(6)} \cos 6\phi + g\mu_B JH \cos(\phi - \phi_H) \} \\ B &= \frac{1}{J} \{ 3B_2^0 J^{(2)} + 15B_6^6 J^{(6)} \cos 6\phi \}. \end{aligned} \quad (5.2.15)$$

If we consider only the zero- and first-order part of the Hamiltonian, i.e. assume  $\mathcal{H} \simeq \mathcal{H}_0 + \mathcal{H}_1$ , it can be brought into diagonal form via two transformations. The first step is to introduce the spatial Fourier transforms of  $\mathcal{J}(ij)$ , eqn (3.4.2), and of  $a_i$ :

$$a_{\mathbf{q}} = \frac{1}{\sqrt{N}} \sum_i a_i e^{-i\mathbf{q} \cdot \mathbf{R}_i} \quad ; \quad a_{\mathbf{q}}^+ = \frac{1}{\sqrt{N}} \sum_i a_i^+ e^{i\mathbf{q} \cdot \mathbf{R}_i}, \quad (5.2.16)$$

for which the commutators are

$$[a_{\mathbf{q}}, a_{\mathbf{q}'}^+] = \frac{1}{N} \sum_i e^{-i(\mathbf{q}-\mathbf{q}') \cdot \mathbf{R}_i} = \delta_{\mathbf{q}\mathbf{q}'}$$

In the case of an hcp lattice, with its two ions per unit cell, the situation is slightly more complex, as discussed in the previous section. However, this complication is inessential in the present context, and for simplicity we consider a Bravais lattice in the rest of this section, so that the results which we obtain are only strictly valid for excitations propagating in

the  $c$ -direction, for which the double-zone representation may be used. Introducing the Fourier transforms, we may write

$$\mathcal{H}_1 = \sum_{\mathbf{q}} \left[ A_{\mathbf{q}} a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} + B \frac{1}{2} (a_{\mathbf{q}}^{\dagger} a_{-\mathbf{q}}^{\dagger} + a_{\mathbf{q}} a_{-\mathbf{q}}) \right], \quad (5.2.17)$$

with

$$A_{\mathbf{q}} = A + J\{\mathcal{J}(\mathbf{0}) - \mathcal{J}(\mathbf{q})\}. \quad (5.2.18)$$

$\mathcal{H}_1$  is quadratic in the Bose operators, and it can be diagonalized by performing a *Bogoliubov transformation*. A new Bose operator  $\alpha_{\mathbf{q}}$  is introduced, such that

$$a_{\mathbf{q}} = u_{\mathbf{q}} \alpha_{\mathbf{q}} - v_{\mathbf{q}} \alpha_{-\mathbf{q}}^{\dagger} \quad ; \quad |u_{\mathbf{q}}|^2 - |v_{\mathbf{q}}|^2 = 1, \quad (5.2.19)$$

in terms of which  $\mathcal{H}_0 + \mathcal{H}_1$  is transformed into

$$\mathcal{H}_0 + \mathcal{H}_1 = U_0 + U_1 + \sum_{\mathbf{q}} E_{\mathbf{q}} \alpha_{\mathbf{q}}^{\dagger} \alpha_{\mathbf{q}}, \quad (5.2.20)$$

when  $u_{\mathbf{q}}$  and  $v_{\mathbf{q}}$  are adjusted appropriately. Here they can both be chosen to be real quantities, and are determined by the equation

$$(u_{\mathbf{q}} \pm v_{\mathbf{q}})^2 = (A_{\mathbf{q}} \pm B)/E_{\mathbf{q}}. \quad (5.2.21)$$

The energy parameters are

$$U_1 = \frac{1}{2} \sum_{\mathbf{q}} (E_{\mathbf{q}} - A_{\mathbf{q}}) \quad ; \quad E_{\mathbf{q}} = \sqrt{A_{\mathbf{q}}^2 - B^2}. \quad (5.2.22)$$

When  $B$  is different from zero, as occurs if either  $B_2^0$  or  $B_6^6$  is non-zero, the product of the  $|J_{iz} = J\rangle = |0\rangle_i$ -states is no longer the (MF) ground state.  $Q_2^0$  and  $Q_6^6$  give rise to couplings between the single-ion states  $|J\rangle$ ,  $|J-2\rangle$  etc. as reflected in the term proportional to  $B$  in (5.2.17). The new ground state established by the Bogoliubov transformation has the energy  $U_0 + U_1$  ( $= U_0 - \sum_{\mathbf{q}} B^2/4E_{\mathbf{q}}$  to leading order in  $B$ ), which is always smaller than  $U_0$ . The admixture of (predominantly) the  $|J-2\rangle$ -state into the ground state implies that the system is no longer fully polarized at  $T = 0$ , as assumed in (5.2.5). Using (5.2.19) and the conditions  $\langle \alpha_{\mathbf{q}} \alpha_{\mathbf{q}} \rangle = \langle \alpha_{\mathbf{q}}^{\dagger} \alpha_{\mathbf{q}}^{\dagger} \rangle = 0$ , whereas

$$\langle \alpha_{\mathbf{q}}^{\dagger} \alpha_{\mathbf{q}} \rangle = n_{\mathbf{q}} = \frac{1}{e^{\beta E_{\mathbf{q}}} - 1} \quad (5.2.23)$$

is the usual Bose population-factor, we find to first order in  $1/J$ :

$$\langle J_z \rangle = \left\langle J - \frac{1}{N} \sum_{\mathbf{q}} a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} \right\rangle = J(1 - m), \quad (5.2.24)$$

with

$$m = \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{J} \langle a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} \rangle = \frac{1}{N} \sum_{\mathbf{q}} m_{\mathbf{q}}$$

and

$$\begin{aligned} m_{\mathbf{q}} &= \frac{1}{J} \langle (u_{\mathbf{q}} \alpha_{\mathbf{q}}^{\dagger} - v_{\mathbf{q}} \alpha_{-\mathbf{q}}) (u_{\mathbf{q}} \alpha_{\mathbf{q}} - v_{\mathbf{q}} \alpha_{-\mathbf{q}}^{\dagger}) \rangle \\ &= \frac{1}{J} \{ u_{\mathbf{q}}^2 n_{\mathbf{q}} + v_{\mathbf{q}}^2 (n_{\mathbf{q}} + 1) \} \\ &= \frac{1}{J} \left\{ \frac{A_{\mathbf{q}}}{E_{\mathbf{q}}} \left( n_{\mathbf{q}} + \frac{1}{2} \right) - \frac{1}{2} \right\}, \end{aligned} \quad (5.2.25)$$

which is positive and non-zero, even when  $n_{\mathbf{q}} = 0$  at  $T = 0$ .

The second-order contribution to the Hamiltonian is

$$\begin{aligned} \mathcal{H}_2 &= \sum_i \left[ B \frac{1}{8J} (a_i^{\dagger} a_i^{\dagger} + a_i a_i) + C_1 a_i^{\dagger} a_i^{\dagger} a_i a_i \right. \\ &\quad \left. + C_2 (a_i^{\dagger} a_i^{\dagger} a_i^{\dagger} a_i + a_i^{\dagger} a_i a_i a_i) + C_3 (a_i^{\dagger} a_i^{\dagger} a_i^{\dagger} a_i^{\dagger} + a_i a_i a_i a_i) \right] \\ &\quad - \frac{1}{4} \sum_{ij} \mathcal{J}(ij) (2a_i^{\dagger} a_j^{\dagger} a_i a_j - a_i^{\dagger} a_j^{\dagger} a_j a_i - a_i^{\dagger} a_i^{\dagger} a_i a_j), \end{aligned} \quad (5.2.26)$$

with

$$\begin{aligned} C_1 &= -\frac{1}{J^2} \left( \frac{3}{2} B_2^0 J^{(2)} - 105 B_6^6 J^{(6)} \cos 6\phi \right) \\ C_2 &= -\frac{1}{J^2} \left( \frac{3}{4} B_2^0 J^{(2)} + \frac{195}{4} B_6^6 J^{(6)} \cos 6\phi \right) \\ C_3 &= \frac{1}{J^2} \frac{15}{4} B_6^6 J^{(6)} \cos 6\phi. \end{aligned} \quad (5.2.27)$$

Introducing the Fourier transforms of the Bose operators in  $\mathcal{H}_2$ , we find straightforwardly that

$$\begin{aligned} i\hbar \partial a_{\mathbf{q}} / \partial t &= [a_{\mathbf{q}}, \mathcal{H}] \simeq [a_{\mathbf{q}}, \mathcal{H}_1 + \mathcal{H}_2] = A_{\mathbf{q}} a_{\mathbf{q}} + B \left( 1 + \frac{1}{4J} \right) a_{-\mathbf{q}}^{\dagger} + \\ &\frac{1}{N} \sum_{\mathbf{k}, \mathbf{k}'} \left[ \left\{ -\mathcal{J}(\mathbf{q} - \mathbf{k}') + \frac{1}{2} \mathcal{J}(\mathbf{k}') + \frac{1}{4} \mathcal{J}(\mathbf{k}) + \frac{1}{4} \mathcal{J}(\mathbf{q}) + 2C_1 \right\} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}'} a_{\mathbf{q} + \mathbf{k} - \mathbf{k}'} \right. \\ &\quad \left. + C_2 \{ 3a_{\mathbf{k}}^{\dagger} a_{-\mathbf{k}'}^{\dagger} a_{\mathbf{q} + \mathbf{k} - \mathbf{k}'} + a_{-\mathbf{k}} a_{\mathbf{k}'} a_{\mathbf{q} + \mathbf{k} - \mathbf{k}'} \} + 4C_3 a_{\mathbf{k}}^{\dagger} a_{-\mathbf{k}'}^{\dagger} a_{-\mathbf{q} - \mathbf{k} + \mathbf{k}'}^{\dagger} \right], \end{aligned} \quad (5.2.28)$$

for the operator  $[a_{\mathbf{q}}, \mathcal{H}]$ , which appears in the equation of motion of, for instance  $\langle \langle a_{\mathbf{q}} ; a_{\mathbf{q}}^{\dagger} \rangle \rangle$ . When the thermal averages of terms due to  $\mathcal{H}_2$

are considered, the replacement of  $\mathcal{H}$  by  $\mathcal{H}_0 + \mathcal{H}_1$  in the density matrix only gives rise to errors of higher-order in  $1/J$ . Because  $\mathcal{H}_0 + \mathcal{H}_1$  is quadratic in the Bose operators, this replacement results in a decoupling of the  $\mathcal{H}_2$ -terms (according to *Wick's theorem*) which is equivalent to the RPA decoupling utilized previously. Hence, when considering thermal averages, we have to leading order in  $1/J$ , for instance,

$$\begin{aligned} a_{\mathbf{k}}^+ a_{\mathbf{k}'} a_{\mathbf{q}+\mathbf{k}-\mathbf{k}'} &\simeq a_{\mathbf{k}}^+ \langle a_{\mathbf{k}'} a_{\mathbf{q}+\mathbf{k}-\mathbf{k}'} \rangle + a_{\mathbf{k}'} \langle a_{\mathbf{k}}^+ a_{\mathbf{q}+\mathbf{k}-\mathbf{k}'} \rangle + a_{\mathbf{q}+\mathbf{k}-\mathbf{k}'} \langle a_{\mathbf{k}} a_{\mathbf{k}'} \rangle \\ &= \delta_{\mathbf{k},-\mathbf{q}} a_{-\mathbf{q}}^+ \langle a_{\mathbf{k}'} a_{-\mathbf{k}'} \rangle + \delta_{\mathbf{k}',\mathbf{q}} a_{\mathbf{q}} \langle a_{\mathbf{k}}^+ a_{\mathbf{k}} \rangle + \delta_{\mathbf{k},\mathbf{k}'} a_{\mathbf{q}} \langle a_{\mathbf{k}}^+ a_{\mathbf{k}} \rangle, \end{aligned} \quad (5.2.29)$$

where the last line follows from the diagonality of  $\mathcal{H}_0 + \mathcal{H}_1$  in reciprocal space. We note that it is convenient here that the single-ion operators are expressed as products of Bose operators which are well-ordered. When this decoupling is introduced in (5.2.28), it reduces to

$$[a_{\mathbf{q}}, \mathcal{H}] = \tilde{A}_{\mathbf{q}}(T) a_{\mathbf{q}} + \tilde{B}_{\mathbf{q}}(T) a_{-\mathbf{q}}^+, \quad (5.2.30)$$

where the effective, renormalized parameters are

$$\begin{aligned} \tilde{A}_{\mathbf{q}}(T) &= A + 4JC_1 m + 6JC_2 b + J\{\mathcal{J}(\mathbf{0}) - \mathcal{J}(\mathbf{k})\}(1 - m) \\ &\quad + \frac{1}{N} \sum_{\mathbf{k}} J\{\mathcal{J}(\mathbf{k}) - \mathcal{J}(\mathbf{k} - \mathbf{q})\} m_{\mathbf{k}} \end{aligned} \quad (5.2.31a)$$

and

$$\begin{aligned} \tilde{B}_{\mathbf{q}}(T) &= B \left(1 + \frac{1}{4J}\right) + 2JC_1 b + 6JC_2 m + 12JC_3 b - \frac{1}{2} J\{\mathcal{J}(\mathbf{0}) - \mathcal{J}(\mathbf{q})\} b \\ &\quad + \frac{1}{2N} \sum_{\mathbf{k}} J\{\mathcal{J}(\mathbf{0}) - \mathcal{J}(\mathbf{k})\} b_{\mathbf{k}} + \frac{1}{N} \sum_{\mathbf{k}} J\{\mathcal{J}(\mathbf{k}) - \mathcal{J}(\mathbf{k} - \mathbf{q})\} b_{\mathbf{k}}. \end{aligned} \quad (5.2.31b)$$

$m_{\mathbf{k}}$  and  $b_{\mathbf{k}}$  are respectively the correlation functions  $(1/J)\langle a_{\mathbf{k}}^+ a_{\mathbf{k}} \rangle$  and  $(1/J)\langle a_{\mathbf{k}}^+ a_{-\mathbf{k}}^+ \rangle = (1/J)\langle a_{\mathbf{k}} a_{-\mathbf{k}} \rangle$ , and  $m$  and  $b$  are the corresponding averages over  $\mathbf{k}$ . Equation (5.2.30) implies that the operator  $[a_{\mathbf{q}}, \mathcal{H}]$ , in the equations of motion of any Green function involving  $a_{\mathbf{q}}$ , can be replaced by the expression on the right-hand side. The same result is obtained if, instead,  $\mathcal{H}_2$  is neglected, and  $A_{\mathbf{q}}$  and  $B$  in  $\mathcal{H}_1$  are replaced by  $\tilde{A}_{\mathbf{q}}(T)$  and  $\tilde{B}_{\mathbf{q}}(T)$  in (5.2.17). Consequently, the system behaves as if the Hamiltonian  $\mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_2$  is replaced by  $\tilde{\mathcal{H}}_0 + \tilde{\mathcal{H}}_1$ , which is similar to  $\mathcal{H}_0 + \mathcal{H}_1$  except for the introduction of the effective, temperature-dependent parameters. The RPA decoupling (5.2.29) introduces errors in the Green functions, but only in the third order of  $1/J$ , and as it leads to an effective Hamiltonian which is quadratic in the Bose operators, it is a valid procedure. This internal consistency of the theory to second order in

$1/J$  means that the RPA contributions to the correlation functions are reliably estimated, and that all second-order contributions are included when  $\tilde{\mathcal{H}}_0 + \tilde{\mathcal{H}}_1$  is used, instead of  $\mathcal{H}_0 + \mathcal{H}_1$ , in the calculation of the thermal averages. We shall therefore use the following self-consistent expressions for the characteristic correlation functions,  $m_{\mathbf{k}}$  and  $b_{\mathbf{k}}$ , determined straightforwardly by utilizing the correspondence between  $\mathcal{H}_0 + \mathcal{H}_1$  and  $\tilde{\mathcal{H}}_0 + \tilde{\mathcal{H}}_1$ :

$$m_{\mathbf{k}} = \frac{1}{J} \left\{ \frac{\tilde{A}_{\mathbf{k}}(T)}{E_{\mathbf{k}}(T)} \left( n_{\mathbf{k}} + \frac{1}{2} \right) - \frac{1}{2} \right\}, \quad (5.2.32a)$$

corresponding to (5.2.25), and

$$b_{\mathbf{k}} = -\frac{1}{J} \frac{\tilde{B}_{\mathbf{k}}(T)}{E_{\mathbf{k}}(T)} \left( n_{\mathbf{k}} + \frac{1}{2} \right). \quad (5.2.32b)$$

In order to express the result in a convenient form, we rewrite one of the second-order terms in  $\tilde{B}_{\mathbf{q}}(T)$  as

$$\frac{1}{2N} \sum_{\mathbf{k}} J \{ \mathcal{J}(\mathbf{0}) - \mathcal{J}(\mathbf{k}) \} b_{\mathbf{k}} = -\frac{1}{2} B \left( m + \frac{1}{2J} \right) - \frac{1}{2} A b + \mathcal{O}(1/J^3), \quad (5.2.33)$$

since, to leading order,  $J \{ \mathcal{J}(\mathbf{0}) - \mathcal{J}(\mathbf{k}) \} = \tilde{A}_{\mathbf{k}}(T) - A$ , and  $\tilde{B}_{\mathbf{k}}(T)$  in  $b_{\mathbf{k}}$  can be approximated by  $B$ . We note that  $A_{\mathbf{q}}$  and  $B$  are parameters of the order  $1/J$ , as are  $m$  and  $b$  (at low temperatures). In addition to introducing (5.2.33) into (5.2.31b), it is adequate for calculating the spin-wave energies to define a transformed set of parameters:

$$\begin{aligned} A_{\mathbf{q}}(T) &= \tilde{A}_{\mathbf{q}}(T) + \frac{1}{2} \tilde{B}_{\mathbf{q}}(T) b \\ B_{\mathbf{q}}(T) &= \tilde{B}_{\mathbf{q}}(T) + \frac{1}{2} \tilde{A}_{\mathbf{q}}(T) b \end{aligned} \quad (5.2.34)$$

and these are then, to the order considered,

$$\begin{aligned} A_{\mathbf{q}}(T) &= A + 4JC_1 m + 6JC_2 b + \frac{1}{2} B b \\ &+ J \{ \mathcal{J}(\mathbf{0}) - \mathcal{J}(\mathbf{q}) \} (1 - m) + \frac{1}{N} \sum_{\mathbf{k}} J \{ \mathcal{J}(\mathbf{k}) - \mathcal{J}(\mathbf{k} - \mathbf{q}) \} m_{\mathbf{k}} \end{aligned} \quad (5.2.35a)$$

and

$$\begin{aligned} B_{\mathbf{q}}(T) &= B + 2JC_1 b + 6JC_2 m + 12JC_3 b - \frac{1}{2} B m \\ &+ \frac{1}{N} \sum_{\mathbf{k}} J \{ \mathcal{J}(\mathbf{k}) - \mathcal{J}(\mathbf{k} - \mathbf{q}) \} b_{\mathbf{k}}. \end{aligned} \quad (5.2.35b)$$

This transformation leaves the expression for the excitation energies unchanged, i.e.

$$E_{\mathbf{q}}(T) = \{ [A_{\mathbf{q}}(T) + B_{\mathbf{q}}(T)][A_{\mathbf{q}}(T) - B_{\mathbf{q}}(T)] \}^{\frac{1}{2}}, \quad (5.2.36)$$



when higher-order corrections are neglected. Inserting the eqns (5.2.15), (5.2.18), and (5.2.27) into (5.2.35), we finally obtain, at zero wave-vector,

$$A_{\mathbf{0}}(T) - B_{\mathbf{0}}(T) = \frac{1}{J} \left\{ -36B_6^6 J^{(6)} (1 - 20m + 15b) \cos 6\phi \right. \\ \left. + g\mu_B JH \cos(\phi - \phi_H) \right\} \quad (5.2.37a)$$

and

$$A_{\mathbf{0}}(T) + B_{\mathbf{0}}(T) = \frac{1}{J} \left\{ 6B_2^0 J^{(2)} (1 - 2m - b) \right. \\ \left. - 6B_6^6 J^{(6)} (1 - 20m + 5b) \cos 6\phi + g\mu_B JH \cos(\phi - \phi_H) \right\}, \quad (5.2.37b)$$

and, at non-zero wave-vector,

$$A_{\mathbf{q}}(T) = A_{\mathbf{0}}(T) + J \{ \mathcal{J}(\mathbf{0}) - \mathcal{J}(\mathbf{q}) \} (1 - m) + \frac{1}{N} \sum_{\mathbf{k}} J \{ \mathcal{J}(\mathbf{k}) - \mathcal{J}(\mathbf{k} - \mathbf{q}) \} m_{\mathbf{k}} \quad (5.2.38a)$$

and

$$B_{\mathbf{q}}(T) = B_{\mathbf{0}}(T) + \frac{1}{N} \sum_{\mathbf{k}} J \{ \mathcal{J}(\mathbf{k}) - \mathcal{J}(\mathbf{k} - \mathbf{q}) \} b_{\mathbf{k}}. \quad (5.2.38b)$$

The spin-wave energies deduced here, to second order in the expansion in  $1/J$ , depend on temperature and on the crystal-field mixing of the  $J_z$ -eigenstates, and both dependences are introduced via the two correlation functions  $m_{\mathbf{k}}$  and  $b_{\mathbf{k}}$ , given self-consistently by (5.2.32) in terms of the energy parameters.  $B_{\mathbf{q}}(T)$  vanishes if there is no anisotropy, i.e. if  $B_2^0$  and  $B_6^6$  are zero. In the case of single-ion anisotropy,  $B_{\mathbf{q}}(T)$  is independent of  $\mathbf{q}$  if the small second-order term in (5.2.38b) is neglected, nor does it depend on the magnetic field, except for the slight field-dependence which may occur via the correlation functions  $m$  and  $b$ .

When the spin-wave excitation energies have been calculated, it is a straightforward matter to obtain the corresponding response functions. Within the present approximation, the  $xx$ -component of the susceptibility is

$$\chi_{xx}(\mathbf{q}, \omega) = -\frac{1}{4N} \sum_{ij} \langle \langle (J_+ + J_-)_i e^{-i\mathbf{q} \cdot \mathbf{R}_i}; (J_+ + J_-)_j e^{i\mathbf{q} \cdot \mathbf{R}_j} \rangle \rangle \\ = -\frac{J}{2} \left( 1 - \frac{1}{2}m - \frac{1}{4}b \right)^2 \langle \langle a_{\mathbf{q}} + a_{-\mathbf{q}}^+; a_{\mathbf{q}}^+ + a_{-\mathbf{q}} \rangle \rangle. \quad (5.2.39)$$

The Bogoliubov transformation, eqns (5.2.19) and (5.2.21), with the parameters replaced by renormalized values, then leads to

$$\chi_{xx}(\mathbf{q}, \omega) = -\frac{J}{2} \left( 1 - m - \frac{1}{2}b \right) \frac{\tilde{A}_{\mathbf{q}}(T) - \tilde{B}_{\mathbf{q}}(T)}{E_{\mathbf{q}}(T)} \langle \langle \alpha_{\mathbf{q}} + \alpha_{-\mathbf{q}}^+; \alpha_{\mathbf{q}}^+ + \alpha_{-\mathbf{q}} \rangle \rangle,$$

which is a simple combination of Bose Green-functions determined by (5.2.20), with  $E_{\mathbf{q}}$  replaced by  $E_{\mathbf{q}}(T)$ . Introducing these functions and the parameters given by (5.2.34), we finally obtain

$$\chi_{xx}(\mathbf{q}, \omega) = J(1-m) \frac{A_{\mathbf{q}}(T) - B_{\mathbf{q}}(T)}{E_{\mathbf{q}}^2(T) - (\hbar\omega)^2}, \quad (5.2.40a)$$

neglecting third-order terms. A rotation of the coordinate system by  $\pi/2$  around the  $z$ -axis changes the sign of  $B_{\mathbf{q}}(T)$ , and hence we have

$$\chi_{yy}(\mathbf{q}, \omega) = J(1-m) \frac{A_{\mathbf{q}}(T) + B_{\mathbf{q}}(T)}{E_{\mathbf{q}}^2(T) - (\hbar\omega)^2}. \quad (5.2.40b)$$

These results show that the ratio between the neutron-scattering intensities due to the spin-wave at  $\mathbf{q}$ , neglecting  $S_{zz}(\mathbf{q}, \omega)$ , in the two cases where the scattering vector is perpendicular to the basal  $y$ - $z$  plane and to the  $x$ - $z$  plane is

$$R_{\mathbf{q}}(T) = \left. \frac{S_{xx}(\mathbf{q}, \omega)}{S_{yy}(\mathbf{q}, \omega)} \right|_{\hbar\omega = \pm E_{\mathbf{q}}(T)} = \frac{\chi_{xx}(\mathbf{q}, 0)}{\chi_{yy}(\mathbf{q}, 0)} = \frac{A_{\mathbf{q}}(T) - B_{\mathbf{q}}(T)}{A_{\mathbf{q}}(T) + B_{\mathbf{q}}(T)}. \quad (5.2.41)$$

The measured intensities from Tb, which differ substantially from those calculated for the Heisenberg ferromagnet, agree well with this expression, especially if the correction for anisotropic two-ion coupling is taken into account (Jensen *et al.* 1975).

In the Heisenberg ferromagnet without rotational anisotropy, corresponding to  $B_{\mathbf{q}}(T) = 0$ , the elementary excitations at low temperatures are *circularly* polarized spin waves, in which the local moments precess in circles around the equilibrium direction. In the presence of anisotropy,  $R_{\mathbf{q}}(T)$  differs from unity, and the excitations become *elliptically* polarized spin waves. The eccentricity of the ellipse depends on the wave-vector of the excited spin wave, and by definition  $R_{\mathbf{q}}(T)$  is the square of the ratio of the lengths of the principal axes which, at least to the order in  $1/J$  which we have considered, is equal to the ratio between the corresponding static susceptibility components. So the static anisotropy is reflected, in a direct way, in the normal modes of the system. The result (5.2.41) justifies the transformation (5.2.34) by attributing observable effects to the parameters  $A_{\mathbf{q}}(T) \pm B_{\mathbf{q}}(T)$ , whereas the parameters which are defined via the Hamiltonian alone, here  $\tilde{A}_{\mathbf{q}}(T) \pm \tilde{B}_{\mathbf{q}}(T)$ , depend on the particular Bose representation which is employed.

The longitudinal correlation function  $S_{zz}(\mathbf{q}, \omega)$ , which is neglected above, contains a diffusive mode at zero frequency, but no well-defined normal modes of non-zero frequency. There is inelastic scattering, but

the inelastic response, as well as the elastic mode, are purely of second order in  $1/J$  and we shall not consider the longitudinal fluctuations further here.

The method developed in this section may be utilized, essentially unchanged, to calculate the MF susceptibility  $\bar{\chi}^o(\omega)$  of the *single* sites. The result to first order in  $1/J$  is:

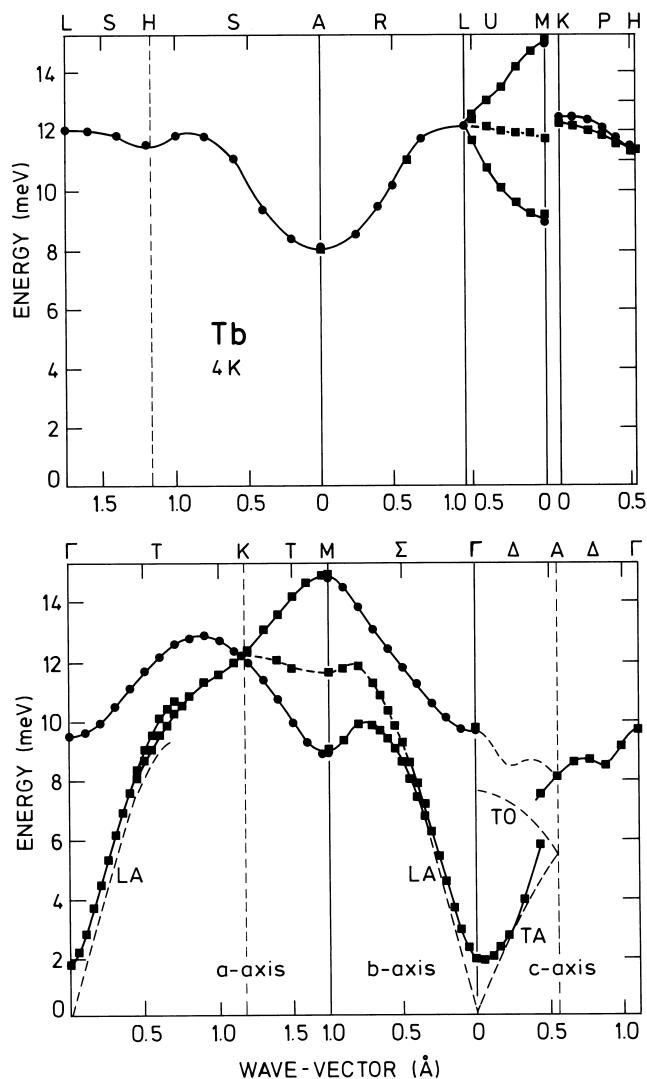
$$\begin{aligned}\chi_{xx}^o(\omega) &= \langle J_z \rangle \frac{A - B + h_{\text{ex}}}{E_{\text{ex}}^2 - (\hbar\omega)^2} \\ \chi_{yy}^o(\omega) &= \langle J_z \rangle \frac{A + B + h_{\text{ex}}}{E_{\text{ex}}^2 - (\hbar\omega)^2} \\ \chi_{xy}^o(\omega) &= -\chi_{yx}^o(\omega) = \langle J_z \rangle \frac{i\hbar\omega}{E_{\text{ex}}^2 - (\hbar\omega)^2},\end{aligned}\tag{5.2.42a}$$

where  $\langle J_z \rangle$  is the MF expectation value of  $J_z$ ,  $h_{\text{ex}}$  is the exchange field, and  $E_{\text{ex}}$  is the energy of the first excited MF state:

$$h_{\text{ex}} = \langle J_z \rangle \mathcal{J}(\mathbf{0}) \quad ; \quad E_{\text{ex}}^2 = (A + h_{\text{ex}})^2 - B^2.\tag{5.2.42b}$$

Introducing this expression for  $\bar{\chi}^o(\omega)$  into the RPA equation (3.5.8), we may derive  $\bar{\chi}(\mathbf{q}, \omega)$  by the same method as was used for the Heisenberg ferromagnet in Section 3.5.2, in which case  $A = B = 0$ . The results for the  $xx$ - and  $yy$ -components are then found to agree with eqn (5.2.40) to leading order in  $1/J$ . To the next order in  $1/J$ , the parameters are replaced by renormalized values, but this procedure is not here easily generalized so as to become fully self-consistent. However, most of the corrections may be included by substituting  $A_{\mathbf{0}}(T) \pm B_{\mathbf{0}}(T)$  for  $A \pm B$  in the expression for  $\bar{\chi}^o(\omega)$ , and the self-consistent value of  $\langle J_z \rangle$  for its MF value. The only terms which are not included in  $\bar{\chi}(\mathbf{q}, \omega)$  by this procedure, as we may see by a comparison with eqn (5.2.40), are the  $\mathbf{q}$ -dependent contributions to  $A_{\mathbf{q}}(T) \pm B_{\mathbf{q}}(T)$  determined by the  $\mathbf{k}$ -sums in (5.2.38). At low temperatures, these contributions are small and may safely be neglected in systems with long-range interactions. This formulation therefore represents a valid alternative, which is useful for generalizing the linear spin-wave theory to the hcp structure, discussed in Section 5.1, or to the helically or conically ordered systems which we will consider in Chapter 6.

As an example of the *magnon dispersion relations* for the anisotropic basal-plane ferromagnet, we show in Fig. 5.2 experimental measurements on Tb at 4K (Mackintosh and Bjerrum Møller 1972). The principal differences between these results and the corresponding excitations for Gd in Fig. 5.1 are the pronounced interactions which are observed between the magnons and phonons, which we shall discuss in some detail in



**Fig. 5.2.** The spin-wave dispersion relations along the symmetry lines in the Brillouin zone for Tb. In contrast to Gd, the anisotropy gives rise to an energy gap at the origin, and there are large effects due to interactions with the phonons. The third branch along, for example,  $\Gamma$ M may also be due to phonon interactions, or it may be a manifestation of the breaking of the hexagonal symmetry by the ordered moment in a particular domain, in the multi-domain sample. The lifting of the double degeneracy along the line KH provides evidence for anisotropic two-ion coupling.

Section 5.4.2, and the appearance of an energy gap at long wavelengths. This gap has its origin in the magnetic anisotropy. Even though the exchange energy required to excite a magnon vanishes in the long-wavelength limit, work is still required to turn the moments away from the easy direction against the anisotropy forces. If we neglect the small terms due to the sums over  $\mathbf{k}$  in (5.2.38), the dispersion relation along the  $c$ -axis in zero field becomes, from eqns (5.2.36–38),

$$E_{\mathbf{q}}(T) = \{ [A_{\mathbf{0}}(T) + B_{\mathbf{0}}(T) + \langle J_z \rangle \{ \mathcal{J}(\mathbf{0}) - \mathcal{J}(\mathbf{q}) \} ] \\ \times [A_{\mathbf{0}}(T) - B_{\mathbf{0}}(T) + \langle J_z \rangle \{ \mathcal{J}(\mathbf{0}) - \mathcal{J}(\mathbf{q}) \} ] \}^{\frac{1}{2}}. \quad (5.2.43)$$

For an arbitrary direction in the zone, this relation is generalized analogously to eqn (5.1.9), giving rise again to acoustic and optical modes. From the dispersion relations, the *magnon density of states* and  $\mathcal{J}(\mathbf{q})$  may readily be determined and hence, by a Fourier transform, the nominal Heisenberg exchange interaction  $\mathcal{J}(ij)$  between moments on different atomic sites (Houmann 1968). The energy gap at zero wave-vector is given by

$$E_{\mathbf{0}}(T) = \{ [A_{\mathbf{0}}(T) + B_{\mathbf{0}}(T)][A_{\mathbf{0}}(T) - B_{\mathbf{0}}(T)] \}^{\frac{1}{2}}, \quad (5.2.44)$$

and as we shall see in the next section, it is proportional to the geometrical mean of the axial- and hexagonal-anisotropy energies. We shall return to the dependence of this energy gap on the temperature and the magnetoelastic effects in the following two sections.