7.4 Spin Waves

We have derived in Sect. 7.2.2 exact eigenstates of the Heisenberg Hamiltonian, which are the so-called "one-magnon states"

$$|\mathbf{k}\rangle = \frac{1}{\hbar\sqrt{2S\,N}}\,S^{-}(\mathbf{k})|0\rangle \tag{7.244}$$

with the eigenenergies

$$E(\mathbf{k}) = E_0(B_0) + g_J\,\mu_B\,B_0 + 2S\,\hbar^2\,(J_0 - J(\mathbf{k})) \tag{7.245}$$

Here $E_0(B_0)$ is the ground state energy of the Heisenberg ferromagnet

$$E_0(B_0) = -N\,\hbar^2\,J_0\,S^2 - N\,g_J\,\mu_B\,B_0\,S \tag{7.246}$$

The excitation energy

$$\hbar\,\omega(\mathbf{k}) = E(\mathbf{k}) - E_0(B_0) \tag{7.247}$$

is ascribed to the quasiparticle which is called the *magnon*. It corresponds to a spin deviation of one unit of angular momentum ($1\hbar$) which is distributed collectively among all the localized spins in the form of a spin wave.

We have introduced in Sect. 7.1.1 the Holstein–Primakoff transformation, using which the Heisenberg Hamiltonian can be expressed as an infinite series of creation and annihilation operators (7.34). If we terminate the series at the bilinear term, then we get a simplified model Hamiltonian (7.39), whose complete set of eigenstates just consists of exactly the one-magnon states (7.244). The model Hamiltonian thus obtained is called the *harmonic approximation* or the *linear spin wave approximation* of the Heisenberg model, whose predictions and the region of validity will be discussed in this section. This is naturally a *low-temperature approximation*, which is exact if no more than one single magnon is excited and therefore would certainly represent an acceptable approximation, if the number of magnons is small, so that the interaction among the magnons can be neglected. Small magnon number, on the other hand, means that the system is still very close to saturation, which in turn requires low temperatures.

7.4.1 Linear Spin Wave Theory for the Isotropic Ferromagnet

We apply the Holstein–Primakoff transformation (7.23), (7.24) and (7.25) to the spin operators of the Heisenberg Hamiltonian and obtain an infinite series of the form (7.34), which we will break after the first non-trivial term:

$$H = E_0(B_0) + \sum_{\mathbf{q}} \hbar\,\omega(\mathbf{q})\, a^{\dagger}_{\mathbf{q}}\, a_{\mathbf{q}} \tag{7.248}$$

$$\hbar\,\omega(\mathbf{q}) = g_J\,\mu_B\,B_0 + 2S\,\hbar^2\,(J_0 - J(\mathbf{q})) \tag{7.249}$$

$a_{\mathbf{q}}$ and $a^{\dagger}_{\mathbf{q}}$ were introduced in (7.30) and (7.31) as the annihilation and creation operators, respectively, for the magnons of the wavevector $\mathbf{q}$. In (7.248), the summation is over all the wavevectors $\mathbf{q}$ of the first Brillouin zone. In this approximation, H describes a system of uncoupled harmonic oscillators. The general eigenstate of this H is a product of one-magnon states (7.244):

$$|\psi\rangle = \prod_{\mathbf{q}} \left(a^{\dagger}_{\mathbf{q}}\right)^{n_{\mathbf{q}}} |0\rangle \tag{7.250}$$

Here $|0\rangle$ is the *magnon vacuum state*. $n_{\mathbf{q}}$ is the number of magnons with the wavevector $\mathbf{q}$ and therefore is not an operator but the eigenvalue of the number operator $\widehat{n}_{\mathbf{q}} = a^{\dagger}_{\mathbf{q}}\, a_{\mathbf{q}}$. The magnon vacuum state means obviously the ferromagnetic saturation. Therefore, the state $a^{\dagger}_{\mathbf{k}}|0\rangle$ is equivalent to the one-magnon state $|\mathbf{k}\rangle$ given in (7.244).

As $a_{\mathbf{q}}$ and $a^{\dagger}_{\mathbf{q}}$ are Bose operators, we have (Problem 7.13)

$$\left[a_{\mathbf{q}}\,,\ \left(a^{\dagger}_{\mathbf{q}}\right)^{n_{\mathbf{q}}}\right]_{-} = n_{\mathbf{q}}\left(a^{\dagger}_{\mathbf{q}}\right)^{n_{\mathbf{q}}-1} \tag{7.251}$$

Using this one can easily show that

$$H|\psi\rangle = \left(E_0(B_0) + \sum_{\mathbf{q}} \hbar\,\omega(\mathbf{q})\, n_{\mathbf{q}}\right)|\psi\rangle \tag{7.252}$$

where the property

$$a_{\mathbf{q}}|0\rangle = 0 \tag{7.253}$$

has been utilized (Problem 7.13). The energy states are therefore uniquely characterized by the magnon occupation numbers $n_{\mathbf{q}}$. We now know the energy eigenvalues and the eigenstates of the Hamiltonian and hence we can calculate the grand canonical partition function Ξ_0 of the magnon gas. Since the magnon number is not constant, in equilibrium at temperature T, the magnon number will be N_T, for which the free energy F is extremal:

$$\left(\frac{\partial F}{\partial T}\right)_T\bigg|_{N=N_T} = 0 \tag{7.254}$$

On the other hand, the left-hand side is the equation for determining the chemical potential μ; that means, μ for magnons is zero. One can calculate Ξ_0 as in (3.56):

$$\begin{aligned}\Xi_0 &= e^{-\beta E_0} \prod_{\mathbf{q}} \sum_{n_{\mathbf{q}}=0}^{\infty} e^{-\beta\hbar\omega(\mathbf{q})\, n_{\mathbf{q}}} \\ &= e^{-\beta E_0} \prod_{\mathbf{q}} \frac{1}{1 - e^{-\beta\hbar\omega(\mathbf{q})}}\end{aligned} \tag{7.255}$$

From this result, we can derive all the interesting quantities, e.g. *average occupation number*

$$\langle \widehat{n}_{\mathbf{q}} \rangle = \langle a^{\dagger}_{\mathbf{q}}\, a_{\mathbf{q}} \rangle = -\frac{1}{\beta} \frac{\partial}{\partial(\hbar\omega(\mathbf{q}))} \ln \Xi_0$$

for which (3.60) is true. From (7.255) follows the expected result that $\langle \widehat{n}_{\mathbf{q}} \rangle$ is nothing but the Bose–Einstein distribution function:

$$\langle \widehat{n}_{\mathbf{q}} \rangle = \frac{1}{exp(\beta\hbar\omega(\mathbf{q})) - 1} \equiv f_{+}(\hbar\omega(\mathbf{q})) \tag{7.256}$$

The *grand canonical potential*

$$\begin{aligned}\Omega(T, B_0) &= -k_B T \ln \Xi_0 \\ &= E_0(B_0) + k_B T \sum_{\mathbf{q}} \ln\left(1 - e^{-\beta\hbar\omega(\mathbf{q})}\right)\end{aligned} \tag{7.257}$$

gives the magnetization of the spin system:

$$\begin{aligned}M(T, B_0) &= -\frac{1}{V}\left(\frac{\partial \Omega}{\partial B_0}\right)_T \\ &= g_J\, \mu_B\, S\, \frac{N}{V} - \frac{k_B T}{V} \sum_{\mathbf{q}} \frac{\beta\, g_J\, \mu_B e^{-\beta\hbar\omega(\mathbf{q})}}{1 - e^{-\beta\hbar\omega(\mathbf{q})}} \\ &= g_J\, \mu_B\, S\, \frac{N}{V}\left(1 - \frac{1}{NS}\sum_{\mathbf{q}} \langle \widehat{n}_{\mathbf{q}} \rangle\right)\end{aligned} \tag{7.258}$$

One has saturation

$$M_0 = g_J\, \mu_B\, S\, \frac{N}{V} \tag{7.259}$$

only when no magnons are excited, i.e. when $\langle \widehat{n}_{\mathbf{q}} \rangle = 0$ for all $\mathbf{q}$. Therefore

$$\frac{M_0 - M(T, B_0)}{M_0} = \frac{1}{NS} \sum_{\mathbf{q}} \frac{1}{exp(\beta\hbar\omega(\mathbf{q})) - 1} \tag{7.260}$$

We know that this expression will be more and more valid as one goes to lower and lower temperatures. Therefore, we want to investigate the behaviour for $T \to 0$ in more detail. First we will convert, as usual, the sum into an integral

$$\begin{aligned} &\sum_{\mathbf{q}} \left(e^{\beta\hbar\omega(\mathbf{q})} - 1\right)^{-1} \\ &= \frac{V}{(2\pi)^3} \int d^3q \sum_{n=0}^{\infty} e^{-n\beta\hbar\omega(\mathbf{q})}\, e^{-\beta\hbar\omega(\mathbf{q})} \\ &= \frac{V}{(2\pi)^3} \sum_{n=1}^{\infty} e^{-n\beta g_J \mu_B B_0} \int d^3q\, e^{-2nS\beta\hbar^2 (J_0 - J(\mathbf{q}))} \end{aligned} \tag{7.261}$$

Since for low temperatures β is very large, in (7.260), specially the small magnon energies $\hbar\omega(\mathbf{q})$ play a role, i.e. those with small wavevector $|\mathbf{q}|$. In such case, we have

$$\begin{aligned} J_0 - J(\mathbf{q}) &= \frac{1}{N} \sum_{i,j} J_{ij} \left(1 - e^{i\mathbf{q}\cdot\mathbf{R}_{ij}}\right) \\ &= \frac{1}{2N} \sum_{i,j} J_{ij} \left(\mathbf{q} \cdot \mathbf{R}_{ij}\right)^2 \equiv \frac{D}{2S\hbar^2}\, q^2 \end{aligned} \tag{7.262}$$

The linear term disappears because $\mathbf{R}_{ij} = -\mathbf{R}_{ji}$. For small $|\mathbf{q}|$, the magnon energies depend quadratically on the wavevector (see also (7.279))

$$\hbar\, \omega(\mathbf{q}) \approx g_J\ \mu_B\ B_0 + D\, q^2 \tag{7.263}$$

We can, without a great error, apply this approximation in (7.261), since in the region where (7.263) is questionable, the integrand in (7.261) is practically zero. For the same reason, one can extend the integration over the first Brillouin zone to the entire $\mathbf{q}$-space:

$$\begin{aligned} \sum_{\mathbf{q}} \langle n_{\mathbf{q}} \rangle &= \frac{V}{2\pi^2} \sum_{n=1}^{\infty} e^{-n\beta g_J \mu_B B_0} \int_0^{\infty} dq\, q^2\, e^{-n\beta D q^2} \\ &= V \left(\frac{k_B T}{4\pi D}\right)^{3/2} \sum_{n=1}^{\infty} \frac{e^{-n\beta g_J \mu_B B_0}}{n^{3/2}} \end{aligned} \tag{7.264}$$

We abbreviate

$$Z_m(x) = \sum_{n=1}^{\infty} \frac{e^{-nx}}{n^m} \tag{7.265}$$

For $x = 0$, this reduces to the Riemann ζ-function (3.76)

$$Z_m(0) = \zeta(m) \tag{7.266}$$

which is available in the tables ($\zeta(3/2) \approx 2.612$). With this, we have the relative magnetization of the spin system at low temperatures as

$$\frac{M_0 - M(T, B_0)}{M_0} = \frac{V}{NS}\left(\frac{k_B T}{4\pi D}\right)^{3/2} Z_{3/2}\,(\beta\, g_J\, \mu_B\, B_0) \tag{7.267}$$

Here we are specially interested in the spontaneous magnetization ($B_0 = 0$) for which we have derived the famous Bloch's $T^{3/2}$ law:

$$\frac{M_0 - M(T, 0)}{M_0} = C_{3/2}\, T^{3/2} \tag{7.268}$$

$$C_{3/2} = \frac{V}{NS}\left(\frac{k_B}{4\pi D}\right)^{3/2} \zeta(3/2) \tag{7.269}$$

This result of the linear spin wave theory is uniquely confirmed by experiment. We recall that the molecular field approximation predicts an exponential approach of the magnetization to its maximum value. For low temperatures, the spin wave theory provides distinctly better results for isotropic ferromagnets.

In passing, we mention that the approximation (7.262) can be easily improved by not restricting oneself to small $|\mathbf{q}|$ but only taking into account nearest neighbour interactions:

$$J(\mathbf{q}) = \frac{1}{N}\sum_{i,j} J_{ij}\, e^{i\mathbf{q}\cdot\mathbf{R}_{ij}} = \sum_{\Delta}^{n.n} J_{0\Delta}\, e^{i\mathbf{q}\cdot\mathbf{R}_{\Delta}} = z\, J_1\, \gamma_{\mathbf{q}} \tag{7.270}$$

z is the number of nearest neighbours, J_1 is the exchange integral between the nearest neighbours and $\gamma_{\mathbf{q}}$ is a structure factor

$$\gamma_{\mathbf{q}} = \frac{1}{z}\sum_{\Delta}^{n.n} e^{i\mathbf{q}\cdot\mathbf{R}_{\Delta}} \tag{7.271}$$

$\gamma_{\mathbf{q}}$ can be easily evaluated, for example, for the three cubic lattices.

(a) *Simple cubic*

$$z = 6; \quad \mathbf{R}_\Delta = \begin{cases} a(\pm 1,\ 0,\ 0) \\ a(0,\ \pm 1,\ 0) \\ a(0,\ 0,\ \pm 1) \end{cases} \tag{7.272}$$

a is the lattice constant.

$$\gamma_{\mathbf{q}}^{sc} = \frac{1}{3}(\cos(q_x a) + \cos(q_y a) + \cos(q_z a)) \tag{7.273}$$

(b) *Body centred cubic*

$$z = 8; \quad \mathbf{R}_\Delta = \frac{a}{2}\,(\pm 1,\ \pm 1,\ \pm 1) \tag{7.274}$$

$$\gamma_{\mathbf{q}}^{bcc} = \cos(\frac{1}{2}q_x a)\cos(\frac{1}{2}q_y a)\cos(\frac{1}{2}q_z a) \tag{7.275}$$

(c) *Face centred cubic*

$$z = 12; \quad \mathbf{R}_\Delta = \begin{cases} \frac{a}{2}(\pm 1,\ \pm 1,\ 0) \\ \frac{a}{2}(\pm 1,\ 0,\ \pm 1) \\ \frac{a}{2}(0,\ \pm 1,\ \pm 1) \end{cases} \tag{7.276}$$

$$\begin{aligned} \gamma_{\mathbf{q}}^{fcc} = \frac{1}{3}\,&[\cos(\frac{1}{2}q_x\ a)\ \cos(\frac{1}{2}q_y\ a) + \cos(\frac{1}{2}q_x\ a)\ \cos(\frac{1}{2}q_z\ a) \\ &+ \cos(\frac{1}{2}q_y\ a)\ \cos(\frac{1}{2}q_z\ a)] \end{aligned} \tag{7.277}$$

For small wavevectors, all the three cubic lattices hold:

$$\gamma_{\mathbf{q}} \approx 1 - \frac{1}{z}\,a^2\,q^2 \tag{7.278}$$

so that

$$\hbar\,\omega(\mathbf{q}) = g_J\ \mu_B\ B_0 + (2S\ J_1\ \hbar^2\ a^2)q^2 \tag{7.279}$$

As a consequence, the constant D introduced in (7.262) for a cubic lattice becomes

$$D = 2S\ J_1\ \hbar^2\ a^2 \tag{7.280}$$

If we calculate the relative magnetization with either (7.273) or (7.275) or (7.277) instead of with (7.262) then we get corrections to the $T^{3/2}$ term which are proportional to $T^{5/2}$, $T^{7/2}$, $\cdots$ [10]:

$$\frac{M_0 - M_s(T)}{M_0} = \frac{1}{S}\left\{\zeta(3/2)\,t^{3/2} + \frac{3\pi}{4}\delta\,\zeta(5/2)\,t^{5/2} + \pi^2\,\delta^2\,\alpha\,\zeta(7/2)\,t^{7/2} + \cdots\right\} \tag{7.281}$$

where t is a renormalized temperature

$$t = \frac{3k_B T}{4\pi\ S\ J_1\ \hbar^2\ z\ \delta} \tag{7.282}$$

and α and δ are structure factors.

$$\begin{array}{lll} \alpha_{sc} = 33/22 & ;\ \alpha_{bcc} = 281/288 & ;\ \alpha_{fcc} = 15/16 \\ \delta_{sc} = 1 & ;\ \delta_{bcc} = 3\cdot 2^{-4/3} & ;\ \delta_{fcc} = 2^{1/3} \end{array} \tag{7.283}$$

The magnetic (internal) energy of the spin wave system is calculated in a completely analogous fashion as the magnetization. With the "isotropic approximation" (7.263) and $B_0 = 0$, we first get

$$\begin{aligned} \sum_{\mathbf{q}} \hbar\omega(\mathbf{q})\ \langle n_{\mathbf{q}}\rangle &= D\sum_{\mathbf{q}} q^2\ \langle n_{\mathbf{q}}\rangle \\ &= \frac{V}{2\pi^2}\ D\sum_{n=1}^{\infty}\int_0^{\infty} dq\ q^4\ e^{-n\beta D q^2} \\ &= \frac{3V\ D}{16\pi^{3/2}}\left(\frac{k_B T}{D}\right)^{5/2}\sum_{n=1}^{\infty}\frac{1}{n^{5/2}} \end{aligned} \tag{7.284}$$

where we have exploited (7.264). This leads to the following energy expression in the region of validity of the spin wave theory:

$$U_{SW} = E_0(B_0 = 0) + \frac{3V\ \zeta(5/2)}{2(4\pi D)^{3/2}}\ (k_B T)^{5/2} \tag{7.285}$$

Thus the magnetic part of the specific heat also obeys a $T^{3/2}$ law,

$$C_{B_0=0}(T) = \left(\frac{\partial U_{SW}}{\partial T}\right)_{B_0=0} = \frac{15}{4}k_B\ V\ \zeta(5/2)\ \left(\frac{k_B T}{4\pi D}\right)^{3/2} \tag{7.286}$$

which is also confirmed experimentally. The improved version of the specific heat analogously to (7.281) reads as

$$C_{B_0=0}(T) = k_B\ N \left\{ \frac{15}{4}\zeta(5/2)\, t^{3/2} + \frac{105\pi}{16}\ \delta\ \zeta(7/2)\, t^{5/2} + \right.$$
$$\left. + \frac{63}{4}\pi^2\ \delta^2\ \alpha\ \zeta(9/2)\, t^{7/2} + \cdots \right\} \tag{7.287}$$

The experimental proof of the quasiparticle magnon is available from neutron scattering. Neutrons exchange energy and momentum with the phonons and magnons in the solid. The corresponding measurements provide, via the energy–momentum laws, the dispersion curves of the spin waves, i.e. the **q**-dependence of the spin wave energies. Dyson [10], by a far-reaching mathematical investigation of the Heisenberg model, confirmed the spin wave theory. He finds that the interaction among the spin waves produces correction terms, the largest one being $\sim T^4$. Therefore, the spin wave result (7.281) which includes the $T^{7/2}$ term is exact even when the interactions are taken into account. The basis for this somewhat surprising fact can be traced to the interaction term (7.47) in the Dyson–Maléev transformation, which is made up of two summands whose effects compensate each other to a large extent.

7.4.2 "Renormalized" Spin Waves

In this section, we want to discuss in a simple form the effect of interaction among spin waves (*non-linear spin wave theory*). The starting point is the Dyson–Maleev transformation (7.42), (7.43) and (7.44) which was introduced in Sect. 7.1.1. Through this transformation, the Heisenberg Hamiltonian takes the form (7.45)

$$H = E_0(B_0) + H_2 + H_4 \tag{7.288}$$

$E_0(B_0)$ is the ground state energy (7.246):

$$H_2 = \sum_{i,j}(g_J\ \mu_B\ B_0\ \delta_{ij} + 2S\ \hbar^2\ (J_0\ \delta_{ij} - J_{ij}))\ \alpha_i\ \alpha_j^\dagger \tag{7.289}$$

$$H_4 = \hbar^2 \sum_{i,j} J_{ij}(\alpha_i \alpha_j^\dagger\, \widehat{n}_j - \widehat{n}_i\, \widehat{n}_j) \tag{7.290}$$

The advantage of the Dyson–Maleev over the Holstein–Primakoff transformation lies in the fact that, in this case, the Hamiltonian consists of a finite number of terms whereas in the other case there are an infinite number of terms. The disadvantage is of course obvious from (7.42) and (7.43): H is not Hermitean any more. One can, however, show [10] that the non-Hermitean operator (7.44) contains all the eigenvalues of the original Heisenberg Hamiltonian plus an infinite number of "unphysical" eigenvalues. In the Dyson's method the unphysical eigenstates are "pushed up" so that at not too high a temperature, they do not play any role in the partition function (the contribution of a state is $\sim exp(-\beta E_n)$). The details of this method cannot be presented here but the reader is referred to the original work of Dyson [10]. We restrict ourselves here to a very much simplified treatment of the spin wave interaction. With

$$\begin{aligned}\alpha_{\mathbf{q}} &= \tfrac{1}{\sqrt{N}} \textstyle\sum_i e^{-i\mathbf{q}\cdot\mathbf{R}_i}\, \alpha_i \\ \alpha^\dagger_{\mathbf{q}} &= \tfrac{1}{\sqrt{N}} \textstyle\sum_i e^{i\mathbf{q}\cdot\mathbf{R}_i}\, \alpha^\dagger_i\end{aligned} \tag{7.291}$$

we will first transform the Hamiltonian into the wavevector representation. H_2 is simple:

$$H_2 = \sum_{\mathbf{q}} \hbar\, \omega(\mathbf{q})\, \alpha^\dagger_{\mathbf{q}}\, \alpha_{\mathbf{q}} \tag{7.292}$$

This represents the free magnon gas which was discussed in the last section. In addition we now have the interaction H_4 (Problem 7.11),

$$H_4 = \frac{\hbar^2}{N} \sum_{\mathbf{q}_1,\cdots\mathbf{q}_4} (J(\mathbf{q}_4) - J(\mathbf{q}_1 - \mathbf{q}_3))\, \delta_{\mathbf{q}_1+\mathbf{q}_2,\mathbf{q}_3+\mathbf{q}_4}\, \alpha^\dagger_{\mathbf{q}_1}\, \alpha^\dagger_{\mathbf{q}_2}\, \alpha_{\mathbf{q}_3}\, \alpha_{\mathbf{q}_4} \tag{7.293}$$

which naturally cannot be handled exactly. We will try to “diagonalize”, in view of the kronecker delta, by taking only such terms for which

$$\mathbf{q}_1 = \mathbf{q}_3; \quad \mathbf{q}_2 = \mathbf{q}_4$$

or

$$\mathbf{q}_1 = \mathbf{q}_4; \quad \mathbf{q}_2 = \mathbf{q}_3$$

holds (*random phase approximation (RPA)*):

$$\begin{aligned}\tilde{H} &= \\ &= E_0(B_0) + \sum_{\mathbf{q}} \left[2S\hbar^2(J_0 - J(\mathbf{q}))\left(1 + \frac{1}{SN}\right) + g_J\mu_B B_0\right] \widehat{n}_{\mathbf{q}} \\ &+ \frac{\hbar^2}{N} \sum_{\mathbf{q}_1,\mathbf{q}_2} (J(\mathbf{q}_1) + J(\mathbf{q}_2) - J(\mathbf{q}_1 - \mathbf{q}_2) - J(0))\widehat{n}_{\mathbf{q}_1}\widehat{n}_{\mathbf{q}_2}\end{aligned} \tag{7.294}$$

The approximation which leads to $\tilde{H}$ appears completely arbitrary. One can, however, show that in the space of one- and two-magnon states, $\tilde{H}$ is exact. We have treated the one-magnon states in Sect. 7.2.2. The problem of two-magnon states can also be exactly solved [11, 12].

From (7.294) one can see that the magnon occupation operator $\widehat{n}_{\mathbf{q}} = \alpha^\dagger_{\mathbf{q}}\, \alpha_{\mathbf{q}}$ commutes with $\tilde{H}$,

$$\left[\tilde{H}\ ,\ \widehat{n}_{\mathbf{q}}\right]_{-}=0 \tag{7.295}$$

so that the eigenstates of $\tilde{H}$ can be classified according to the occupation numbers $n_{\mathbf{q}}$:

$$|n_{\mathbf{q}_1},\ n_{\mathbf{q}_2},\ \ldots,\ n_{\mathbf{q}_N}\rangle$$

Let a state be given with a particular fixed magnon distribution. Then we ask ourselves what is the energy required to add an additional magnon to the system. That is relatively easy to find out. Let

$$\begin{aligned}\tilde{H}|\cdots n_{\mathbf{q}}\cdots\rangle &= E(n_{\mathbf{q}})|\cdots n_{\mathbf{q}}\cdots\rangle\\ \tilde{H}|\cdots n_{\mathbf{q}}+1\cdots\rangle &= E(n_{\mathbf{q}}+1)|\cdots n_{\mathbf{q}}+1\cdots\rangle\end{aligned} \tag{7.296}$$

Then, we can define the *renormalized spin wave energy*, renormalized by the "presence" of other magnons:

$$\hbar\tilde{\omega}(\mathbf{q})=E(n_{\mathbf{q}}+1)-E(n_{\mathbf{q}}) \tag{7.297}$$

With

$$\left[\widehat{n}_{\mathbf{q}_1}\ ,\ \alpha^{\dagger}_{\mathbf{q}}\right]_{-}=\delta_{\mathbf{q},\mathbf{q}_1}\ \alpha^{\dagger}_{\mathbf{q}} \tag{7.298}$$

and

$$\begin{aligned}\left[\widehat{n}_{\mathbf{q}_1}\,\widehat{n}_{\mathbf{q}_2}\ ,\ \alpha^{\dagger}_{\mathbf{q}}\right]_{-} &= \delta_{\mathbf{q}\mathbf{q}_2}\widehat{n}_{\mathbf{q}_1}\alpha^{\dagger}_{\mathbf{q}}+\delta_{\mathbf{q}\mathbf{q}_1}\alpha^{\dagger}_{\mathbf{q}}\,\widehat{n}_{\mathbf{q}_2}\\ &= \delta_{\mathbf{q}\mathbf{q}_2}\alpha^{\dagger}_{\mathbf{q}}\,\widehat{n}_{\mathbf{q}_1}+\delta_{\mathbf{q}\mathbf{q}_1}\alpha^{\dagger}_{\mathbf{q}}\,\widehat{n}_{\mathbf{q}_2}+\delta_{\mathbf{q}\mathbf{q}_2}\delta_{\mathbf{q}\mathbf{q}_1}\ \alpha^{\dagger}_{\mathbf{q}}\end{aligned} \tag{7.299}$$

from (7.294) it follows that

$$\begin{aligned}\left[\tilde{H}\ ,\ \alpha^{\dagger}_{\mathbf{q}}\right]_{-} &= \hbar\,\omega(\mathbf{q})\,\alpha^{\dagger}_{\mathbf{q}}\\ &\quad+\frac{2\hbar^2}{N}\sum_{\mathbf{q}_1}(J(\mathbf{q})+J(\mathbf{q}_1)-J(\mathbf{q}-\mathbf{q}_1)-J(0))\,\alpha^{\dagger}_{\mathbf{q}}\,\widehat{n}_{\mathbf{q}_1}\end{aligned} \tag{7.300}$$

We can now directly show that $\alpha^{\dagger}_{\mathbf{q}}|\cdots n_{\mathbf{q}}\cdots\rangle$ is an eigenstate for the magnon number $n_{\mathbf{q}}+1$. With (7.298) it holds that

$$\begin{aligned}\widehat{n}_{\mathbf{q}}\left(\alpha^{\dagger}_{\mathbf{q}}|\cdots n_{\mathbf{q}}\cdots\rangle\right) &= \left(\alpha^{\dagger}_{\mathbf{q}}\,\widehat{n}_{\mathbf{q}}+\alpha^{\dagger}_{\mathbf{q}}\right)|\cdots n_{\mathbf{q}}\cdots\rangle\\ &= \left(n_{\mathbf{q}}+1\right)\left(\alpha^{\dagger}_{\mathbf{q}}|\cdots n_{\mathbf{q}}\cdots\rangle\right)\end{aligned}$$

That means

$$\alpha_{\mathbf{q}}^{\dagger}|\cdots n_{\mathbf{q}}\cdots\rangle \sim |\cdots n_{\mathbf{q}}+1\cdots\rangle \tag{7.301}$$

The operation of $\tilde{H}$ on this state gives the eigenvalue $E(n_{\mathbf{q}}+1)$:

$$\tilde{H}\left(\alpha_{\mathbf{q}}^{\dagger}|\cdots n_{\mathbf{q}}\cdots\rangle\right) = E(n_{\mathbf{q}}+1)\left(\alpha_{\mathbf{q}}^{\dagger}|\cdots n_{\mathbf{q}}\cdots\rangle\right) \tag{7.302}$$

On the other hand, we have from (7.300)

$$\begin{aligned}\tilde{H}\left(\alpha_{\mathbf{q}}^{\dagger}|\cdots n_{\mathbf{q}}\cdots\rangle\right) &= \alpha_{\mathbf{q}}^{\dagger}\,\tilde{H}|\cdots n_{\mathbf{q}}\cdots\rangle + \left[\tilde{H}\;,\;\alpha_{\mathbf{q}}^{\dagger}\right]_{-}|\cdots n_{\mathbf{q}}\cdots\rangle \\ &= \Big\{E(n_{\mathbf{q}}) + \hbar\,\omega(\mathbf{q}) + \\ &+ \frac{2\hbar^2}{N}\sum_{\mathbf{q}_1}(J(\mathbf{q}) + J(\mathbf{q}_1) - J(\mathbf{q}-\mathbf{q}_1) \\ &-\; J(0))n_{\mathbf{q}_1}\Big\}\left(\alpha_{\mathbf{q}}^{\dagger}|\cdots n_{\mathbf{q}}\cdots\rangle\right)\end{aligned} \tag{7.303}$$

Equations (7.302) and (7.303) give via (7.297) the *renormalized spin wave energies*:

$$\hbar\,\tilde{\omega}(\mathbf{q}) = \hbar\,\omega(\mathbf{q}) + \frac{2\hbar^2}{N}\sum_{\mathbf{q}_1}(J(\mathbf{q}) + J(\mathbf{q}_1) - J(\mathbf{q}-\mathbf{q}_1) - J(0))\,n_{\mathbf{q}_1} \tag{7.304}$$

The sum therefore represents the correction to the linear spin wave theory due to the magnon interactions. The sum contains the occupation numbers $n_{\mathbf{q}_1}$ of the magnons which can in principle be an arbitrarily large integer number which can apparently lead to unphysical states. The $\{n_{\mathbf{q}}\}$ are naturally uniquely fixed by the state $|\cdots n_{\mathbf{q}}\cdots\rangle$. We are interested in the spin wave energies which appear in the thermodynamic equilibrium. Therefore, it is reasonable to replace $n_{\mathbf{q}_1}$ by its thermodynamic expectation value which we assume is given by Bose-distribution function.

$$n_{\mathbf{q}_1} \to \langle\widehat{n}_{\mathbf{q}_1}\rangle = \{exp(\beta\,\hbar\,\tilde{\omega}(\mathbf{q}_1)) - 1\}^{-1} \tag{7.305}$$

This leads to an implicit equation for the "renormalized" spin wave energies:

$$\hbar\,\tilde{\omega}(\mathbf{q}) = \hbar\,\omega(\mathbf{q}) + \frac{2\hbar^2}{N}\sum_{\mathbf{q}_1}\frac{J(\mathbf{q}) + J(\mathbf{q}_1) - J(\mathbf{q}-\mathbf{q}_1) - J(0)}{exp(\beta\,\hbar\,\tilde{\omega}(\mathbf{q}_1)) - 1} \tag{7.306}$$

We want to evaluate this expression wherein, as in (7.270), we will restrict ourselves to the nearest neighbour interactions:

$$J(\mathbf{q}) = z\,J_1\,\gamma_{\mathbf{q}};\quad J_0 = z\,J_1 \tag{7.307}$$

By exploiting the translational symmetry of the lattice one can demonstrate that (Problem 7.17)

$$\sum_{\mathbf{q}_1} \gamma_{\mathbf{q}-\mathbf{q}_1} \, \langle \widehat{n}_{\mathbf{q}_1} \rangle \approx \gamma_{\mathbf{q}} \sum_{\mathbf{q}_1} \gamma_{\mathbf{q}_1} \, \langle \widehat{n}_{\mathbf{q}_1} \rangle \tag{7.308}$$

With this (7.306) simplifies to ($B_0 = 0$)

$$\begin{aligned} \hbar\, \tilde{\omega}(\mathbf{q}) = 2S\, \hbar^2\, z\, J_1(1-\gamma_{\mathbf{q}}) - \\ - \frac{2\hbar^2}{N}\, z\, J_1(1-\gamma_{\mathbf{q}}) \sum_{\mathbf{q}_1} (1-\gamma_{\mathbf{q}_1}) \langle \widehat{n}_{\mathbf{q}_1} \rangle \end{aligned}$$

We define

$$A_s(T) = \frac{1}{NS} \sum_{\mathbf{q}_1} (1-\gamma_{\mathbf{q}_1}) \langle \widehat{n}_{\mathbf{q}_1} \rangle \tag{7.309}$$

and obtain an expression for the "renormalized" spin waves which is formally identical to the one for free spin waves:

$$\hbar\, \tilde{\omega}(\mathbf{q}) = 2S\, \hbar^2\, J_0^*(T)(1-\gamma_{\mathbf{q}}) \tag{7.310}$$

We only have to replace the exchange constant J_0 by a temperature-dependent quantity

$$J_0^*(T) = J_0(1 - A_s(T)) \tag{7.311}$$

The summation over the wavevectors of the first Brillouin zone needed in calculating $A_s(T)$ in (7.309) can be evaluated exactly for cubic lattices. We will, however, give only an estimate of $A_s(T)$ which is correct in the limit of small $|\mathbf{q}|$:

$$\hbar\, \tilde{\omega}(\mathbf{q}) \approx D(T)\, q^2 \tag{7.312}$$

$$D(T) = D(1 - A_s(T)) \tag{7.313}$$

$$D = 2S\, J_1\, \hbar^2\, a^2 \tag{7.314}$$

Then correspondingly according to (7.278)

$$1 - \gamma_{\mathbf{q}} \approx \frac{1}{z}\, a^2\, q^2 \tag{7.315}$$

holds. We substitute this in (7.309):

$$
\begin{aligned}
A_s(T) &\approx \frac{a^2}{zNS} \sum_{\mathbf{q}} \frac{q^2}{exp(\beta D(T) q^2) - 1} \\
&= \frac{a^2}{zNS} \frac{V}{(2\pi)^3} \int_{1st\ BZ} d^3q\ q^2 \sum_{n=1}^{\infty} e^{-n\beta D(T) q^2}
\end{aligned} \tag{7.316}
$$

Because of the exponential function in the integrand, we can extend the **q**-integration over the entire **q**-space. This assumption is especially reasonable, because of β in the exponent, in the low-temperature region.

$$
\begin{aligned}
A_s(T) &\approx \frac{a^2\ V}{2\pi^2\ zNS} \sum_{n=1}^{\infty} \int_0^{\infty} dq\ q^4\ e^{-n\beta D(T) q^2} \\
&= \frac{a^2\ V}{2\pi^2\ zNS} \sum_{n=1}^{\infty} \frac{3}{8}\sqrt{\pi} \left(\frac{k_B T}{nD(T)}\right)^{5/2} \\
&= 3\frac{a^2\ V}{16\pi^{3/2}\ zNS} \left(\frac{k_B T}{D(T)}\right)^{5/2}\ \zeta(5/2)
\end{aligned} \tag{7.317}
$$

This equation along with (7.313) fixes $A_s(T)$. Let us write

$$
\eta = 3\frac{a^2 V}{16\pi^{3/2} zNS} \left(\frac{k_B}{D}\right)^{5/2}\ \zeta(5/2)
$$

to get as an intermediate result

$$
A_s(T) \approx \eta \left(\frac{T}{1 - A_s(T)}\right)^{5/2}
$$

For low temperatures $A_s(T)$ will be only a small correction term:

$$
\begin{aligned}
A_s(T) &\approx \eta\ T^{5/2} \left(1 + \frac{5}{2} A_s(T) + \cdots\right) \\
&\approx \eta\ T^{5/2} \left(1 + \frac{5}{2} \eta\ T^{5/2} + \cdots\right) = \eta\ T^{5/2} + \mathcal{O}(T^5)
\end{aligned}
$$

This means for the renormalized exchange constant

$$
J_0^*(T) = J_0 \left(1 - \eta\ T^{5/2}\right) \tag{7.318}
$$

If this expression is used in the Bloch's $T^{3/2}$ law of the linear spin wave theory (7.268), then we obtain a T^4 term as a first correction in complete agreement with the exact theory. This can be seen as follows: The constant $C_{3/2}$ (7.269) as the prefactor of the $T^{3/2}$ term has to be renormalized:

$$
\begin{aligned}
C_{3/2} \to C^*_{3/2} &= \frac{V}{NS}\left(\frac{k_B}{4\pi D(T)}\right)^{3/2} \zeta(3/2) \\
&\approx C_{3/2}\left(1 - \eta\, T^{5/2}\right)^{-3/2} \\
&\approx C_{3/2}\left(1 + \frac{3}{2}\eta\, T^{5/2} + \cdots\right) \\
&\approx C_{3/2} + C_4\, T^{5/2} + \cdots
\end{aligned}
$$

This yields for the magnetization, in complete agreement with Dyson's result,

$$
\begin{aligned}
\frac{M_0 - M_s(T)}{M_0} &= C_{3/2}T^{3/2} + C_{5/2}T^{5/2} + C_{7/2}T^{7/2} \\
&\quad + C_4 T^4 + C_{9/2}T^{9/2} + \cdots
\end{aligned}
$$

It was shown that using the renormalized spin wave theory presented here, the magnetization curves of classical ferromagnets like EuO and EuS can be almost quantitatively reproduced up to in the neighbourhood of T_C [13, 14]. In the case of europium chalcogenides, one should not restrict oneself to the nearest neighbour exchange integrals but should also consider the next nearest neighbours. Instead of (7.310) we have to use

$$
\begin{aligned}
\hbar\,\tilde{\omega}(\mathbf{q}) &= 2S\,\hbar^2\, z_1\, J_1(1 - A_1(T))(1 - \gamma_{\mathbf{q}}^{(1)}) \\
&\quad + 2S\,\hbar^2\, z_2\, J_2(1 - A_2(T))(1 - \gamma_{\mathbf{q}}^{(2)})
\end{aligned} \tag{7.319}
$$

z_1 and z_2 are the number of nearest and next nearest neighbours, respectively, and J_1 and J_2 the corresponding exchange integrals.

$$
\gamma_{\mathbf{q}}^{(i)} = \frac{1}{z_i}\sum_{\Delta_i} e^{i\mathbf{q}\cdot\mathbf{R}_{\Delta_i}} \quad (i = 1,\ 2) \tag{7.320}
$$

The sum runs over the nearest (Δ_1) or the next nearest (Δ_2) neighbours, respectively, of the lattice site under consideration.

$$
A_i(T) = \frac{1}{NS}\sum_{\mathbf{q}} \frac{1 - \gamma_{\mathbf{q}}^{(i)}}{exp(\beta\hbar\tilde{\omega}(\mathbf{q})) - 1} \quad (i = 1,\ 2) \tag{7.321}
$$

The integration over the first Brillouin zone (fcc in the case of EuO and EuS) can be exactly performed. In doing this, for EuO and EuS one has to use the following parameters (neutron scattering experiments):

$S = 7/2$

EuO: $\hbar^2\ J_1/k_B = 0.625$ K EuS: $\hbar^2\ J_1/k_B = 0.221$ K

$\hbar^2\ J_2/k_B = 0.125$ K $\hbar^2\ J_2/k_B = -0.100$ K

The agreement between the experimentally determined magnetization curves and the calculated ones using the renormalized spin wave theory and the parameters given above is practically exact in the temperature range of 0 to $0.7T_C$.

One can use either the spin wave result (7.260) or the corresponding result of the renormalized spin wave theory

$$\frac{M_0 - M_s(T)}{M_0} = \frac{1}{NS}\sum_{\mathbf{q}} \frac{1}{e^{\beta\hbar\tilde{\omega}(\mathbf{q})} - 1}$$

in order to make a rough estimate of the Curie temperature. For $T = T_C$, by definition, the magnetization is zero. If one expands the exponential function in the denominator up to the linear term, then one is left with

$$k_B\ T_C = \left\{\frac{1}{NS}\sum_{\mathbf{q}} \frac{1}{\hbar\ \tilde{\omega}(\mathbf{q})}\right\}^{-1} \tag{7.322}$$

The sum can be explicitly evaluated for simple lattices. If one restricts the exchange interaction among the nearest neighbours, one can with (7.273), (7.275) and (7.277) obtain the following values:

$$k_B\ T_C = 2S^2\ \hbar^2\ J_0^*(T_C)\ Q \tag{7.323}$$

where the structure factor Q is given by

$$Q \equiv \left(\frac{1}{N}\sum_{\mathbf{q}} \frac{1}{1-\gamma_{\mathbf{q}}}\right)^{-1} = \begin{cases} 0.660 : \text{sc} \\ 0.718 : \text{bcc} \\ 0.744 : \text{fcc} \end{cases}$$

For estimations this is quite a useful formula. Nevertheless, one has to be cautious about using this result since it follows from the renormalized spin wave theory, which conceptually is naturally a low-temperature approximation, and therefore the T_C obtained is questionable.

7.4.3 Harmonic Approximation for Antiferromagnets

The spin wave approximation has proved itself to be extraordinarily successful in the case of ferromagnets. The same thing cannot be expected for the cases of antiferromagnets and ferrimagnets without certain limitations. In fact, it is not even clear from the beginning whether the idea of spin waves can be taken over to the case of antiferromagnets. In contrast to the ferromagnets, the exact ground state of an antiferromagnet is known only for the one-dimensional lattice (with $S = 1/2$ or $S \to \infty$). If we accept the sub-lattice model (see Sect. 7.3.2), which has been supported by neutron scattering experiments, then the expected ground state (Neel state) is the state in which all the sub-lattices are ferromagnetically saturated. We will, however, be able to show in this section that a completely ordered state cannot be the correct ground state. With an in principle unknown ground state, one cannot talk of elementary excitations without putting some question marks on them. In spite of this, the spin wave theory, in the case of antiferromagnets also, has proved to be a useful approximate analysis. Numerical estimates, concerning the accuracy of the approximation, for a series of reference systems have established the theory to be quite reliable.

Here we want to discuss the simplest form of antiferromagnets, i.e. the ABAB structure (see Sect. 7.3.2) wherein every atom of a sub-lattice has only the atoms of the other sub-lattice as its nearest neighbours. Further, we will restrict ourselves to exchange interaction only between the nearest neighbours. Then we naturally have

$$J_1 < 0 \tag{7.324}$$

Let the external field $\mathbf{B}_0$ be along the "easy" direction, which we also take to be the z-axis. The anisotropy, which defines the "easy" direction is taken into account through an anisotropy field $\mathbf{B}_A$ (7.61):

$$\begin{aligned} H = &-\sum_{i,j}^{n.n} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j - g_J \frac{\mu_B}{\hbar}(B_0 + B_A)\sum_i^A S_i^z \\ &- g_J \frac{\mu_B}{\hbar}(B_0 - B_A)\sum_i^B S_i^z \end{aligned} \tag{7.325}$$

We will use the Holstein–Primakoff transformation (7.23), (7.24) and (7.25) of the spin operators in the *harmonic approximation*:

Sub-lattice A:

$$\frac{1}{\hbar}\, S_i^+ = \sqrt{2S}\, a_i \;\; ; \;\; \frac{1}{\hbar}\, S_i^- = \sqrt{2S}\, a_i^\dagger \;\; ; \;\; \frac{1}{\hbar}\, S_i^z = S - a_i^\dagger\, a_i \tag{7.326}$$

Sub-lattice B:

$$\frac{1}{\hbar}\, S_i^+ = \sqrt{2S}\, b_j^\dagger \;\; ; \;\; \frac{1}{\hbar}\, S_j^- = \sqrt{2S}\, b_j \;\; ; \;\; \frac{1}{\hbar}\, S_j^z = -S + b_j^\dagger\, b_j \tag{7.327}$$

All a-operators commute with all b-operators. For the sake of convenience, b_j and $b_j^\dagger$ are used for the sub-lattice B in place of the usual definition (7.24) and (7.25).

We will introduce certain abbreviations:

$$b_A = -2z\, J_1\, \hbar^2\, S + g_J\, \mu_B (B_0 + B_A) \tag{7.328}$$

$$b_B = -2z\, J_1\, \hbar^2\, S - g_J\, \mu_B (B_0 - B_A) \tag{7.329}$$

$$E_a(B_0) = -N\, g_J\, \mu_B\, S\, B_A + N\, z\, J_1\, \hbar^2\, S^2 = E_a \tag{7.330}$$

E_a is the energy of the totally ordered Neel state. The *harmonic approximation* for the operator (7.325) consists of neglecting the terms which are not bilinear in the magnon operators. By substituting (7.326) and (7.327) in (7.325) one obtains, retaining bilinear terms only

$$\begin{aligned} H = {} & E_a + b_A \sum_i^A a_i^\dagger\, a_i + b_B \sum_j^B b_j^\dagger\, b_j \\ & - 2S\hbar^2 \sum_i^A \sum_j^B J_{ij} (a_i\, b_j + a_i^\dagger\, b_j^\dagger) \end{aligned} \tag{7.331}$$

We now transform again into the wavevectors $\mathbf{q}$ which are from the first Brillouin zone of each sub-lattice. Since the two sub-lattices are identical, so are the Brillouin zones:

$$a_i = \sqrt{\frac{2}{N}} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{R}_i}\, a_{\mathbf{q}} \tag{7.332}$$

$$b_j = \sqrt{\frac{2}{N}} \sum_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{R}_j}\, b_{\mathbf{q}} \tag{7.333}$$

$$J(\mathbf{q}) = \frac{2}{N} \sum_i^A \sum_j^B J_{ij} e^{-i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)}$$

$$\delta_{\mathbf{q},\mathbf{q}'} = \frac{2}{N} \sum_i^A e^{i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{R}_i} = \frac{2}{N} \sum_j^B e^{i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{R}_j} \tag{7.334}$$

In transforming (7.325), however, we will have to remove the restriction of limiting to nearest neighbours. Then one obtains

$$H = E_a + b_A \sum_{\mathbf{q}} a_{\mathbf{q}}^\dagger\, a_{\mathbf{q}} + b_B \sum_{\mathbf{q}} b_{\mathbf{q}}^\dagger\, b_{\mathbf{q}} + \sum_{\mathbf{q}} c(\mathbf{q}) \{a_{\mathbf{q}}\, b_{\mathbf{q}} + a_{\mathbf{q}}^\dagger\, b_{\mathbf{q}}^\dagger\} \tag{7.335}$$

where

$$c(\mathbf{q}) = -2J(\mathbf{q})\,\hbar^2\,S \;\rightarrow\; -2z\,J_1\,\hbar^2\,S\,\gamma_{\mathbf{q}} \tag{7.336}$$

with $\gamma_{\mathbf{q}}$ given by (7.271). The situation is not quite as simple as in the case of ferromagnets since H is not diagonal in a's and b's. Therefore, as a next step, we look for a unitary transformation that diagonalizes H:

$$H = \tilde{E}_a(B_0) + \sum_{\mathbf{q}} \hbar\,\omega_\alpha(\mathbf{q})\,\alpha_{\mathbf{q}}^\dagger\,\alpha_{\mathbf{q}} + \sum_{\mathbf{q}} \hbar\,\omega_\beta(\mathbf{q})\,\beta_{\mathbf{q}}^\dagger\,\beta_{\mathbf{q}} \tag{7.337}$$

$\tilde{E}_a$ is the "true" ground state energy if $\omega_{\alpha,\beta}(\mathbf{q}) \geq 0$. For the "new" operators, we make the ansatz

$$\begin{aligned} \alpha_{\mathbf{q}} &= c_1\,a_{\mathbf{q}} + c_2\,b_{\mathbf{q}}^\dagger \\ \beta_{\mathbf{q}} &= d_1\,a_{\mathbf{q}}^\dagger + d_2\,b_{\mathbf{q}} \end{aligned} \tag{7.338}$$

and demand that the α's and β's fulfil the usual Bose commutation relations:

$$\left[\alpha_{\mathbf{q}}\,,\;\alpha_{\mathbf{q}'}^\dagger\right]_- = \delta_{\mathbf{q}\mathbf{q}'} \;\Leftrightarrow\; |c_1|^2 - |c_2|^2 = 1 \tag{7.339}$$

$$\left[\beta_{\mathbf{q}}\,,\;\beta_{\mathbf{q}'}^\dagger\right]_- = \delta_{\mathbf{q}\mathbf{q}'} \;\Leftrightarrow\; -|d_1|^2 + |d_2|^2 = 1 \tag{7.340}$$

$$\left[\alpha_{\mathbf{q}}\,,\;\beta_{\mathbf{q}'}\right]_- = 0 \;\Leftrightarrow\; c_1\,d_1 = c_2\,d_2 \tag{7.341}$$

With these commutation relations, one can easily see that

$$\left[\alpha_{\mathbf{q}}\,,\;H\right]_- = \hbar\,\omega_\alpha(\mathbf{q})\,\alpha_{\mathbf{q}} = \hbar\,\omega_\alpha(\mathbf{q})(c_1\,a_{\mathbf{q}} + c_2\,b_{\mathbf{q}}^\dagger) \tag{7.342}$$

According to (7.335) it also holds that

$$\begin{aligned} \left[\alpha_{\mathbf{q}}\,,\;H\right]_- &= c_1\,\left[a_{\mathbf{q}}\,,\;H\right]_- + c_2\,\left[b_{\mathbf{q}}^\dagger\,,\;H\right]_- \\ &= c_1\{b_A\,a_{\mathbf{q}} + c(\mathbf{q})\,b_{\mathbf{q}}^\dagger\} \\ &\quad + c_2\{-b_B\,b_{\mathbf{q}}^\dagger - c(\mathbf{q})\,a_{\mathbf{q}}\} \end{aligned} \tag{7.343}$$

By equating the last two equations, we get

$$\begin{aligned} &a_{\mathbf{q}}\,[c_1\,\hbar\,\omega_\alpha(\mathbf{q}) - c_1\,b_A + c_2\,c(\mathbf{q})] \\ &+ b_{\mathbf{q}}^\dagger\,[c_2\,\hbar\,\omega_\alpha(\mathbf{q}) + c_2\,b_B - c_1\,c(\mathbf{q})] = 0 \end{aligned} \tag{7.344}$$

The operators $a_{\mathbf{q}}$ and $b_{\mathbf{q}}^\dagger$ act in different spaces. Therefore, each of the coefficients by itself should be equal to zero. We then obtain the following homogeneous system of equations:

$$\begin{aligned} c_1\,(\hbar\,\omega_\alpha(\mathbf{q}) - b_A) + c_2\,c(\mathbf{q}) &= 0 \\ c_1\,(-c(\mathbf{q})) + c_2(\hbar\,\omega_\alpha(\mathbf{q}) + b_B) &= 0 \end{aligned} \tag{7.345}$$

whose coefficients-determinant must vanish:

$$(\hbar\omega_\alpha(\mathbf{q}) - b_A)(\hbar\omega_\alpha(\mathbf{q}) - b_B) = -c^2(\mathbf{q})$$

This condition is satisfied through

$$\hbar\,\omega_\alpha(\mathbf{q}) = \frac{1}{2}\left[b_A - b_B + \sqrt{(b_A + b_B)^2 - 4c^2(\mathbf{q})}\,\right] \tag{7.346}$$

The solution with negative square root, which in principle is present, is excluded on physical grounds. This is because the excitations must always be positive even for $B_0 = 0$. However, according to (7.328) and (7.329), for $B_0 = 0$, the first summand $(b_A - b_B)$ is zero.

Completely analogously, if we start with $[\beta_{\mathbf{q}}\ ,\ H]_-$ instead of $[\alpha_{\mathbf{q}}\ ,\ H]_-$ in (7.343) we get

$$\hbar\,\omega_\beta(\mathbf{q}) = \frac{1}{2}\left[b_B - b_A + \sqrt{(b_A + b_B)^2 - 4c^2(\mathbf{q})}\,\right] \tag{7.347}$$

By substituting for the abbreviations b_A and b_B the full expressions according to (7.328) and (7.329) we get the following for the excitation energies for spin waves in an antiferromagnet:

$$\begin{aligned}\hbar\,\omega_\pm(\mathbf{q}) = {}&\sqrt{4S^2\hbar^4(J_0^2 - J^2(\mathbf{q})) + g_J\mu_B B_A(g_J\mu_B B_A - 4SJ_0\hbar^2)}\\ &\pm g_J\mu_B B_0\end{aligned} \tag{7.348}$$

This spectrum differs from that of a ferromagnet in a characteristic manner:

1. There are *two* spin wave branches which in the presence of a field show a constant, i.e. $\mathbf{q}$-independent splitting, and are degenerate for $B_0 = 0$.
2. The minimum spin wave energy is for $\mathbf{q} = \mathbf{0}$. This leads for $B_0 = 0$ to an *energy gap* E_g in the spin wave spectrum, which is typical for antiferromagnets.

$$E_g = \sqrt{g_J\ \mu_B\ B_A(g_J\ \mu_B\ B_A - 4S\ J_0\ \hbar^2)} \tag{7.349}$$

   E_g is determined by the anisotropy field B_A and also by the exchange J_0 ($J_0 = z\ J_1\ <\ 0$). As a result, E_g can be of considerable magnitude. It is obvious that this energy gap, when k_BT is smaller or comparable to E_g, can influence decisively thermodynamic quantities such as the susceptibility, specific heat and sub-lattice magnetization. For $T\ <\ E_g/k_B$, the spin waves are *frozen* and the quantities mentioned depend exponentially on temperature.
3. From (7.348) one sees that the spin wave branch $\hbar\ \omega_-(\mathbf{q})$ can have negative values for fields

$$B_0 \geq B_0^* = E_g/g_J\ \mu_B. \tag{7.350}$$

This is a signature of the instability of the system since it is possible to have excitations of arbitrarily high order with a gain in energy. This is the collapse of the spin wave approximation. The system itself avoids this collapse by going over to a different spin configuration. B_0^* corresponds to the spin-flop field B_F (7.217) of the molecular field approximation. The sub-lattice magnetizations, which were originally either parallel or antiparallel to the easy axis, now orient themselves perpendicular to the field (see Fig. 7.11). From this one recognizes how important the anisotropy field is for the stabilization of antiferromagnets.

4. In the absence of field according to (7.348) the spin wave energy of an antiferromagnet is doubly degenerate:

$$\hbar\,\omega_0(\mathbf{q}) = \sqrt{E_g^2 + 4S^2\,\hbar^4(J_0^2 - J^2(\mathbf{q}))} \tag{7.351}$$

If we assume in addition only a small anisotropy then

$$\hbar\,\omega_0(\mathbf{q}) \approx 2S\,\hbar^2\sqrt{(J_0 + J(\mathbf{q}))(J_0 - J(\mathbf{q}))} \tag{7.352}$$

If we further restrict ourselves to small $|\mathbf{q}|$, then using (7.270) and (7.278) we can write

$$(J_0 + J(\mathbf{q})) \approx 2J_0; \quad (J_0 - J(\mathbf{q})) \approx \frac{1}{z}\,a^2\,q^2\,J_0$$

This leads to a linear $\mathbf{q}$-dependence of the spin wave energy of an antiferromagnet:

$$\hbar\,\omega(\mathbf{q}) \approx \left(2S\,\hbar^2\,|J_0|\,a\,\sqrt{\frac{2}{z}}\right)q \tag{7.353}$$

This is different from that of a ferromagnet, which has for small $|\mathbf{q}|$ a quadratic q-dependence. A direct consequence of the linear q-dependence is a T^3 law at low temperatures of the specific heat (Problem 7.14) which is in contrast to the $T^{3/2}$ dependence (7.286) of the specific heat of a ferromagnet. In case the anisotropy is dominant so that E_g is very large, then we again get a quadratic q-dependence:

$$\begin{aligned}\hbar\,\omega_0(\mathbf{q}) &\approx E_g + \frac{2S^2\,\hbar^4}{E_g}(J_0^2 - J^2(\mathbf{q})) \\ &\approx E_g + \left(\frac{4S^2\,J_0^2\,\hbar^4\,a^2}{z\,E_g}\right)q^2\end{aligned} \tag{7.354}$$

Then there are modifications of the T^3 behaviour.

For a further discussion of antiferromagnets, it appears meaningful to specify the transformation (7.338) more precisely. This is connected with the *Bogoliubov transformation* which is known from the theory of superconductivity. The conditions

(7.339), (7.340) and (7.341) on the coefficients $c_{1,2}$ and $d_{1,2}$ of the transformation can obviously be fulfilled through the following ansatz:

$$\begin{aligned} c_1 &= \cosh \eta_{\mathbf{q}}; \quad & c_2 &= -\sinh \eta_{\mathbf{q}} \\ d_1 &= -\sinh \eta_{\mathbf{q}}; \quad & d_2 &= \cosh \eta_{\mathbf{q}} \end{aligned} \tag{7.355}$$

$\eta_{\mathbf{q}}$ is fixed by the system of equations (7.345)

$$\tanh \eta_{\mathbf{q}} = -\frac{c_2}{c_1} = \frac{\hbar\, \omega_\alpha(\mathbf{q}) - b_A}{c(\mathbf{q})}$$

Substituting (7.346) we get

$$\begin{aligned} \tanh 2\eta_{\mathbf{q}} &= \frac{2 \tanh \eta_{\mathbf{q}}}{1 + \tanh \eta_{\mathbf{q}}} \\ &= 2c(\mathbf{q}) \frac{\hbar\omega(\mathbf{q}) - b_A}{c^2(\mathbf{q}) + (\hbar\omega(\mathbf{q}) - b_A)^2} \\ &= -\frac{2c(\mathbf{q})}{b_A + b_B} \\ &= \frac{2\hbar^2\, S\, J(\mathbf{q})}{g_J\, \mu_B\, B_A - 2\hbar^2\, S\, J_0} \end{aligned} \tag{7.356}$$

An extremely interesting quantity is the energy constant $\tilde{E}_a(B_0)$ appearing in the transformed Hamiltonian (7.337) which represents the true ground state energy of the spin system in the spin wave approximation. So far we have not calculated it explicitly. For doing this, we first use the inverse transformation to (7.338):

$$\begin{aligned} a_{\mathbf{q}} &= \bar{c}_1\, \alpha_{\mathbf{q}} + \bar{c}_2\, \beta_{\mathbf{q}}^{\dagger} \\ b_{\mathbf{q}} &= \bar{d}_1\, \alpha_{\mathbf{q}}^{\dagger} + \bar{d}_2\, \beta_{\mathbf{q}} \end{aligned} \tag{7.357}$$

$$\bar{c}_1 = \bar{d}_2 = \cosh\ \eta_{\mathbf{q}}; \quad \bar{c}_2 = \bar{d}_1 = \sinh\ \eta_{\mathbf{q}} \tag{7.358}$$

which we insert in the "original" Hamiltonian (7.335). This naturally results again in (7.337) since the transformation was conceptualized precisely for this purpose. In addition, we obtain the "new" energy constant

$$\tilde{E}_a(B_0) = E_a - \frac{N}{4}(b_A + b_B) + \frac{1}{2}\sum_{\mathbf{q}} \sqrt{(b_A + b_B)^2 - 4c^2(\mathbf{q})} = \tilde{E}_a \tag{7.359}$$

We perform the explicit transformation as Problem 7.16.

This is an extremely interesting result which shows that the ground state energy $\tilde{E}_a$ is smaller than the energy E_a of the fully ordered Neel state, in which the sub-lattice magnetizations are oriented exactly antiparallel to each other. One should recognize that the difference

$$\tilde{E}_a - E_a = -\frac{N}{2}(-2J_0\,\hbar^2\,S + g_J\,\mu_B\,B_A) + \sum_{\mathbf{q}}\sqrt{E_g^2 + 4S^2\,\hbar^4(J_0^2 - J^2(\mathbf{q}))} \leq 0 \tag{7.360}$$

is independent of field. The fully ordered Neel state is certainly not the ground state of the antiferromagnet, which has to possess some spin disorder which should be noticeable in the sub-lattice magnetizations. Therefore, as a next step, they should be calculated.

According to (7.326), for the magnetization of the sub-lattice A

$$M_A = \frac{1}{V}\,\frac{g_J\,\mu_B}{\hbar}\sum_{i=1}^{N/2}\langle S_i^z\rangle_A = \frac{N}{2V}\,g_J\,\mu_B\,S - \frac{1}{V}\,g_J\,\mu_B\sum_i\langle a_i^\dagger\,a_i\rangle$$

holds. When we transform into the wavenumbers, we have to evaluate

$$M_A = \frac{1}{V}\,g_J\,\mu_B\left(\frac{N}{2}\,S - \sum_{\mathbf{q}}\langle a_{\mathbf{q}}^\dagger\,a_{\mathbf{q}}\rangle\right) \tag{7.361}$$

We exploit (7.357):

$$\langle a_{\mathbf{q}}^\dagger\,a_{\mathbf{q}}\rangle = \bar{c}_1^2\langle\alpha_{\mathbf{q}}^\dagger\,\alpha_{\mathbf{q}}\rangle + \bar{c}_2^2\langle\beta_{\mathbf{q}}\;\;\beta_{\mathbf{q}}^\dagger\rangle + \bar{c}_1\,\bar{c}_2\left(\langle\alpha_{\mathbf{q}}^\dagger\,\beta_{\mathbf{q}}^\dagger\rangle + \langle\beta_{\mathbf{q}}\,\alpha_{\mathbf{q}}\rangle\right)$$

According to (7.337), in the linear spin wave approximation, the quasiparticles created by $\alpha_{\mathbf{q}}$ and $\beta_{\mathbf{q}}$ represent a fully decoupled system in which the particle number is conserved. That means, e.g.

$$\langle\alpha_{\mathbf{q}}^\dagger\,\beta_{\mathbf{q}}^\dagger\rangle = \langle\beta_{\mathbf{q}}\alpha_{\mathbf{q}}\rangle = 0 \tag{7.362}$$

so that

$$\langle a_{\mathbf{q}}^\dagger\,a_{\mathbf{q}}\rangle = \cosh^2\eta_{\mathbf{q}}\,\langle\alpha_{\mathbf{q}}^\dagger\,\alpha_{\mathbf{q}}\rangle + \sinh^2\eta_{\mathbf{q}}(1 + \langle\beta_{\mathbf{q}}^\dagger\,\beta_{\mathbf{q}}\rangle) \tag{7.363}$$

The α- and β-quasiparticles are non-interacting Bosons ($\mu = 0$). Therefore, the expectation values of their occupation number operators on the right-hand side of (7.363) are the Bose–Einstein distribution functions:

$$M_A = \frac{1}{V}\, g_J\, \mu_B \left[\left(\frac{N}{2}\, S - \sum_{\mathbf{q}} \sinh^2 \eta_{\mathbf{q}} \right) - \right.$$
$$\left. - \sum_{\mathbf{q}} \left(\frac{\cosh^2 \eta_{\mathbf{q}}}{exp(\beta\, \hbar\, \omega_\alpha(\mathbf{q})) - 1} + \frac{\sinh^2 \eta_{\mathbf{q}}}{exp(\beta\, \hbar\, \omega_\beta(\mathbf{q})) - 1} \right) \right] \tag{7.364}$$

With

$$\begin{aligned} \cosh^2 \eta_{\mathbf{q}} &= \frac{1}{2} \left[1 + \left(\sqrt{1 - \tanh^2 2\eta_{\mathbf{q}}} \right)^{-1} \right] \\ \sinh^2 \eta_{\mathbf{q}} &= \frac{1}{2} \left[-1 + \left(\sqrt{1 - \tanh^2 2\eta_{\mathbf{q}}} \right)^{-1} \right] \end{aligned} \tag{7.365}$$

(7.356) for $\tanh 2\eta_{\mathbf{q}}$ and (7.346) and (7.347) for $\hbar\omega_\alpha$ and $\hbar\omega_\beta$, the temperature dependence of the sub-lattice magnetization in the spin wave region is fully determined. We are particularly interested in the $T = 0$ *sub-lattice magnetization*

$$M_A(T = 0) = \frac{1}{V}\, g_J\, \mu_B \left(\frac{N}{2}\, S - \sum_{\mathbf{q}} \sinh^2 \eta_{\mathbf{q}} \right) \tag{7.366}$$

The first summand corresponds to the complete orientation of the spins (Neel state) whereas the second corresponds to the fluctuations mentioned earlier which are not obviously visualizable. Let us set

$$M_A(T = 0) = \frac{N}{2V}\, g_J\, \mu_B (S - \sigma) \tag{7.367}$$

Then the correction σ can be easily evaluated for simple lattices if we assume the anisotropies $B_A = 0$ in (7.356):

$$\sigma = \frac{1}{N} \sum_{\mathbf{q}} \left(\frac{J_0}{\sqrt{J_0^2 - J^2(\mathbf{q})}} - 1 \right) \tag{7.368}$$

For the NaCl structure for which the whole lattice is simple cubic and the interpenetrating sub-lattices are fcc, one finds [15]

$$\sigma = 0.078 \tag{7.369}$$

That is a typical order of magnitude. The correction term is not too large but not negligible, either, especially for $S = 1/2$.

For the magnetization of the sub-lattice B (7.327) analogous to (7.361) holds:

$$M_B = \frac{1}{V} g_J \, \mu_B \left(-\frac{N}{2} S + \sum_{\mathbf{q}} \langle b_{\mathbf{q}}^{\dagger} \, b_{\mathbf{q}} \rangle \right) \tag{7.370}$$

where now we have to set

$$\langle b_{\mathbf{q}}^{\dagger} \, b_{\mathbf{q}} \rangle = \sinh^2 \eta_{\mathbf{q}} (1 + \langle \alpha_{\mathbf{q}}^{\dagger} \, \alpha_{\mathbf{q}} \rangle) + \cosh^2 \eta_{\mathbf{q}} \langle \beta_{\mathbf{q}}^{\dagger} \, \beta_{\mathbf{q}} \rangle$$

With this we get for the total magnetization

$$\begin{aligned} M(T, B_0) &= M_A(T, B_0) + M_B(T, B_0) \\ &= -\frac{1}{V} g_J \, \mu_B \sum_{\mathbf{q}} \left(\langle \alpha_{\mathbf{q}}^{\dagger} \, \alpha_{\mathbf{q}} \rangle - \langle \beta_{\mathbf{q}}^{\dagger} \, \beta_{\mathbf{q}} \rangle \right) \end{aligned} \tag{7.371}$$

The fluctuation terms of the two sub-lattices thus cancel out. For $B_0 = 0$, naturally $\hbar \, \omega_\alpha = \hbar \, \omega_\beta$ and therefore also $\langle \alpha_{\mathbf{q}}^{\dagger} \, \alpha_{\mathbf{q}} \rangle = \langle \beta_{\mathbf{q}}^{\dagger} \, \beta_{\mathbf{q}} \rangle$ so that the total magnetization vanishes.

At the end we now calculate the *susceptibility* of the antiferromagnet. For that we expand the magnetization up to the linear term in B_0. For $B_0 = 0$ the spin waves $\hbar\omega_\alpha$ and $\hbar\omega_\beta$ are according to (7.351) identical to $\hbar\omega_0$.

$$\begin{aligned} \langle \alpha_{\mathbf{q}}^{\dagger} \, \alpha_{\mathbf{q}} \rangle &= [exp(\beta\hbar\omega_\alpha(\mathbf{q})) - 1]^{-1} \\ &= \langle \alpha_{\mathbf{q}}^{\dagger} \, \alpha_{\mathbf{q}} \rangle^{(0)} - \beta g_J \mu_B B_0 \frac{exp(\beta\hbar\omega_0)}{(exp(\beta\hbar\omega_0) - 1)^2} + \mathcal{O}(B^2) \end{aligned}$$

A completely analogous expression is obtained for $\langle \beta_{\mathbf{q}}^{\dagger} \, \beta_{\mathbf{q}} \rangle$ which along with $\langle \alpha_{\mathbf{q}}^{\dagger} \, \alpha_{\mathbf{q}} \rangle$ we substitute in (7.371). Then the field dependence of the total magnetization reads as

$$M(T, B_0) = \frac{2}{V} \, \beta (g_J \mu_B)^2 \, B_0 \sum_{\mathbf{q}} \frac{exp(\beta\hbar\omega_0(\mathbf{q}))}{(exp(\beta\hbar\omega_0(\mathbf{q})) - 1)^2} + \mathcal{O}(B_0^2) \tag{7.372}$$

With this we directly get for the susceptibility

$$\chi_{\parallel}(T) = \frac{2\mu_0}{V} \, \beta (g_J \mu_B)^2 \sum_{\mathbf{q}} \frac{exp(\beta\hbar\omega_0(\mathbf{q}))}{(exp(\beta\hbar\omega_0(\mathbf{q})) - 1)^2} \tag{7.373}$$

7.4.4 Harmonic Approximation for a Ferromagnet with Dipolar Interaction

In this section we want to discuss the effect of dipole interaction on the spin wave spectrum of a ferromagnet. In the last section we have seen that the fully ordered spin state is not the ground state of an antiferromagnet. In contrast, in the case of *isotropic* ferromagnet, the ground state is indicated by a complete parallel alignment of the localized spins (7.108). However, this is no more correct even for a ferromagnet as soon as we introduce anisotropy which leads to additional terms in the Hamiltonian which do not commute with the z-component of the total spin $S^z = \sum_i S_i^z$. One example for this is the dipole interaction between the localized magnetic moments, which, in particular for ferromagnets with low transition temperatures (EuS!), should not be neglected. According to (7.50), we have to take the dipole interaction into account by including the following additional term in the Hamiltonian:

$$H_D = \sum_{i,j} D_{ij} \left\{ \mathbf{S}_i \cdot \mathbf{S}_j - 3(\mathbf{S}_i \cdot \mathbf{e}_{ij})(\mathbf{S}_j \cdot \mathbf{e}_{ij}) \right\} \tag{7.374}$$

$$D_{ii} = 0; \quad D_{ij} = \frac{\mu_0}{8\pi} \frac{g_J^2 \, \mu_B^2}{\hbar^2 |\mathbf{R}_i - \mathbf{R}_j|^3} \quad (i \neq j) \tag{7.375}$$

$$\mathbf{e}_{ij} = \frac{\mathbf{R}_i - \mathbf{R}_j}{|\mathbf{R}_i - \mathbf{R}_j|} \equiv (x_{ij}, \; y_{ij}, \; z_{ij}) \tag{7.376}$$

The dipole interaction is surely of much smaller significance compared to the exchange interaction but at the same time it has much longer range. Through the second summand in (7.374) it leads to an anisotropy which can be important in many practical applications.

We split the model Hamiltonian into an isotropic (H_i) and an anisotropic part (H_a):

$$H = H_i + H_a \tag{7.377}$$

The isotropic part is different from the model discussed in Sect. 7.4.1 only by the renormalization of the coupling constants:

$$H_i = -\sum_{i,j} (J_{ij} - D_{ij})(S_i^+ \, S_j^- + S_i^z \, S_j^z) - g_J \frac{\mu_B}{\hbar} B_0 \sum_i S_i^z \tag{7.378}$$

What is new is the anisotropy part:

$$H_a = -3 \sum_{i,j} D_{ij} (\mathbf{S}_i \cdot \mathbf{e}_{ij})(\mathbf{S}_j \cdot \mathbf{e}_{ij}) \tag{7.379}$$

For the spin operators we again use the Holstein–Primakoff transformation (7.23), (7.24) and (7.25) in the "harmonic approximation":

$$\frac{1}{\hbar}\, S_i^+ = \sqrt{2S}\, a_i; \quad \frac{1}{\hbar}\, S_i^- = \sqrt{2S}\, a_i^\dagger; \quad \frac{1}{\hbar}\, S_i^z = S - a_i^\dagger\, a_i \tag{7.380}$$

Defining

$$D_0 = \sum_i D_{ij} = \sum_j D_{ij} \tag{7.381}$$

$$b_0 = g_J\, \mu_B\, B_0 + 2S\, \hbar^2\, (J_0 - D_0) \tag{7.382}$$

$$E_0(B_0) = -g_J\, \mu_B\, B_0\, N\, S - \hbar^2 (J_0 - D_0) N\, S^2 \tag{7.383}$$

we get almost directly for the isotropic part of the Hamiltonian

$$H_i = E_0(B_0) + b_0 \sum_i n_i - 2S\, \hbar^2 \sum_{i,j} (J_{ij} - D_{ij}) a_i\, a_j^\dagger \tag{7.384}$$

In obtaining this we have, in the spirit of the harmonic approximation, left out all the terms which are not bilinear in the magnon construction operators a_i, $a_i^\dagger$. The anisotropic part of the dipole interaction H_a possesses somewhat more difficulties. One finds (Problem 7.19)

$$\begin{aligned} H_a = &-3S^2\, \hbar^2 \sum_{i,j} D_{ij}\, z_{ij}^2 \\ &- 3S\, \hbar^2 \sum_{i,j} D_{ij} \Bigg[(x_{ij}^2 + y_{ij}^2) a_i^\dagger\, a_j + \frac{1}{2} (x_{ij} - i y_{ij})^2 a_i\, a_j \\ &+ \frac{1}{2} \left(x_{ij} + i y_{ij} \right)^2 a_i^\dagger\, a_j^\dagger - 2 z_{ij}^2\, n_i \Bigg] \end{aligned} \tag{7.385}$$

The first term is a c-number which we can absorb in E_0

$$\widehat{E}_0(B_0) = E_0(B_0) - 3S^2\, \hbar^2 \sum_{i,j} D_{ij}\, z_{ij}^2 \tag{7.386}$$

A first diagonalization of the Hamiltonian is obtained by going to the wavenumbers. We define

$$B(\mathbf{q}) = -\frac{3}{2}\, S\, \hbar^2\, \frac{1}{N} \sum_{i,j} D_{ij} (x_{ij} - i y_{ij})^2 e^{i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)} \tag{7.387}$$

$$A(\mathbf{q}) = b_0 + 6S\,\hbar^2 \sum_{i,j} D_{ij}\, z_{ij}^2 - \\ - 2S\,\hbar^2\, \frac{1}{N} \sum_{i,j} \left(J_{ij} + \frac{1}{2}\, D_{ij}(1 - 3z_{ij}^2) \right) e^{i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)} \tag{7.388}$$

and then have

$$H = \widehat{E}_0(B_0) + \sum_{\mathbf{q}} A(\mathbf{q})\, a_{\mathbf{q}}^{\dagger}\, a_{\mathbf{q}} + \\ + \sum_{\mathbf{q}} \left(B(\mathbf{q})\, a_{\mathbf{q}}\, a_{-\mathbf{q}} + B^*(\mathbf{q})\, a_{\mathbf{q}}^{\dagger}\, a_{-\mathbf{q}}^{\dagger} \right) \tag{7.389}$$

Because of the anisotropy $B(\mathbf{q})$, H is not yet diagonal. Just as in the case of antiferromagnets we now take H through the Bogoliubov transformation to the form

$$H = E_1(B_0) + \sum_{\mathbf{q}} \hbar\, \omega_D(\mathbf{q})\, \alpha_{\mathbf{q}}^{\dagger}\, \alpha_{\mathbf{q}} \tag{7.390}$$

For that, for the new operators we make the ansatz:

$$\alpha_{\mathbf{q}} = c_{\mathbf{q}}\, a_{\mathbf{q}} + d_{\mathbf{q}}\, a_{-\mathbf{q}}^{\dagger} \tag{7.391}$$

The fulfilment of the fundamental Bose commutator rules is ensured by the following conditions on the coefficients $c_{\mathbf{q}}$ and $d_{\mathbf{q}}$:

$$\begin{aligned} |c_{\mathbf{q}}|^2 - |d_{\mathbf{q}}|^2 &= 1 \\ c_{\mathbf{q}}\, d_{-\mathbf{q}} - d_{\mathbf{q}}\, c_{-\mathbf{q}} &= 0 \end{aligned} \tag{7.392}$$

Further calculational procedure is similar to that followed for determining the spin wave energies of antiferromagnets.

$$\begin{aligned} \left[\alpha_{\mathbf{q}}\,,\ H\right]_- &= \hbar\, \omega_D(\mathbf{q})\, \alpha_{\mathbf{q}} = \hbar\, \omega_D(\mathbf{q})(c_{\mathbf{q}}\, a_{\mathbf{q}} + d_{\mathbf{q}}\, a_{-\mathbf{q}}^{\dagger}) \\ &= c_{\mathbf{q}} \left[a_{\mathbf{q}}\,,\ H\right]_- + d_{\mathbf{q}} \left[a_{-\mathbf{q}}^{\dagger}\,,\ H\right]_- \\ &= c_{\mathbf{q}} \left(A(\mathbf{q})\, a_{\mathbf{q}} + B^*(\mathbf{q})\, a_{-\mathbf{q}}^{\dagger} + B^*(-\mathbf{q})\, a_{-\mathbf{q}}^{\dagger} \right) + \\ &+ d_{\mathbf{q}} \left(-A(-\mathbf{q})\, a_{-\mathbf{q}}^{\dagger} - B(-\mathbf{q})\, a_{\mathbf{q}} - B(\mathbf{q}) a_{\mathbf{q}} \right) \end{aligned}$$

With $B(\mathbf{q}) = B(-\mathbf{q})$ and $A(\mathbf{q}) = A(-\mathbf{q})$ it further follows that

$$a_{\mathbf{q}} \left\{ c_{\mathbf{q}}\, \hbar\, \omega_D(\mathbf{q}) - c_{\mathbf{q}}\, A(\mathbf{q}) + 2d_{\mathbf{q}}\, B(\mathbf{q}) \right\} + \\ + a_{-\mathbf{q}}^{\dagger} \left\{ d_{\mathbf{q}}\, \hbar\, \omega_D(\mathbf{q}) - 2c_{\mathbf{q}}\, B^*(\mathbf{q}) + d_{\mathbf{q}}\, A(\mathbf{q}) \right\} = 0$$

This equation can only be satisfied when each coefficient by itself is equal to zero. This gives a homogeneous system of equations:

$$\begin{aligned} c_{\mathbf{q}}\,(\hbar\,\omega_D(\mathbf{q}) - A(\mathbf{q})) + d_{\mathbf{q}}\,2B(\mathbf{q}) = 0 \\ c_{\mathbf{q}}\,2B^*(\mathbf{q}) + d_{\mathbf{q}}(-\hbar\,\omega_D(\mathbf{q}) - A(\mathbf{q})) = 0 \end{aligned} \tag{7.393}$$

whose solvability condition

$$-(\hbar\,\omega_D(\mathbf{q}))^2 + A^2(\mathbf{q}) - 4|B(\mathbf{q})|^2 = 0$$

determines the spin wave energies:

$$\hbar\,\omega_D(\mathbf{q}) = \sqrt{A^2(\mathbf{q}) - 4|B(\mathbf{q})|^2} \tag{7.394}$$

Due to the long range of the dipole interaction, the lattice sums needed to calculate $A(\mathbf{q})$ and $B(\mathbf{q})$ are not easy to perform. However, it is in principle quite possible to do it for not too complicated lattices. We will not attempt to do it here in detail [16].

The energy constant $E_1(B_0)$, which obviously according to (7.390) represents the ground state energy of a ferromagnet with dipole interaction, provides many interesting conclusions. First we obtain using (7.393) with (7.392) for the coefficients of the transformation (7.393)

$$|c_{\mathbf{q}}|^2 = \frac{1}{2}\left(\frac{A(\mathbf{q})}{\hbar\,\omega_D(\mathbf{q})} + 1\right); \quad |d_{\mathbf{q}}|^2 = \frac{1}{2}\left(\frac{A(\mathbf{q})}{\hbar\,\omega_D(\mathbf{q})} - 1\right) \tag{7.395}$$

where the phase remains free for the moment. This will be uniquely determined from the condition that the Hamiltonian (7.389) takes the form (7.390) after the transformation. For that we invert the transformation (7.391)

$$a_{\mathbf{q}} = c^*_{\mathbf{q}}\,\alpha_{\mathbf{q}} - d_{\mathbf{q}}\,\alpha^\dagger_{-\mathbf{q}} \tag{7.396}$$

and use this in (7.389). H will be diagonal only when we fix the phase as follows:

$$B(\mathbf{q}) = |B(\mathbf{q})|\,e^{i\phi};\ \ c_{\mathbf{q}} = |c_{\mathbf{q}}|\,e^{-i\phi/2};\ \ d_{\mathbf{q}} = |d_{\mathbf{q}}|\,e^{i\phi/2} \tag{7.397}$$

With this we finally get the energy constant $E_1(B_0)$ in (7.390):

$$E_1(B_0) = \widehat{E}_0(B_0) - \frac{1}{2}\sum_{\mathbf{q}}\{A(\mathbf{q}) - \hbar\,\omega_D(\mathbf{q})\} \tag{7.398}$$

$\widehat{E}_0(B_0)$ is the energy of the fully ordered ferromagnet. From

$$E_1(B_0) < \widehat{E}_0(B_0) \tag{7.399}$$

we must conclude as in the case of an antiferromagnet that due to the anisotropy part in the dipole interaction (7.379), the fully ordered spin state is not the ground state of a ferromagnet any more.

Finally we have also described a ferromagnet with dipole interaction by a system of non-interacting bosons. For the quantities such as the partition function, the average occupation density, the grand canonical potential and the internal energy, formally the same relations are valid as for an isotropic ferromagnet. We only have to replace $\hbar\omega(\mathbf{q})$ by $\hbar\omega_D(\mathbf{q})$ everywhere:

$$\Xi(T, B_0) = exp(-\beta\ E_1(B_0)) \prod_{\mathbf{q}} \frac{1}{1 - exp(\beta\hbar\omega_D(\mathbf{q}))} \tag{7.400}$$

$$\langle n(\mathbf{q})\rangle = [exp(\beta\hbar\omega_D(\mathbf{q})) - 1]^{-1} \tag{7.401}$$

$$\begin{aligned} \Omega(T, B_0) = E_1(B_0) + \\ + k_B T \sum_{\mathbf{q}} \ln(1 - exp(-\beta\hbar\omega_D(\mathbf{q}))) \end{aligned} \tag{7.402}$$

$$U = E_1(B_0) + \sum_{\mathbf{q}} \hbar\omega_D(\mathbf{q})\langle n(\mathbf{q})\rangle \tag{7.403}$$

While calculating the *magnetization*

$$M(T, B_0) = -\frac{1}{V}\left(\frac{\partial\Omega}{\partial B_0}\right)_T \tag{7.404}$$

we have to pay attention to the fact that $A(\mathbf{q})$ depends on B_0 whereas $B(\mathbf{q})$ does not. With (7.383), (7.386) and (7.398), the following holds for the energy constant:

$$\frac{\partial E_1(B_0)}{\partial B_0} = -g_J\ \mu_B\ N\ S - \frac{1}{2}\ g_J\ \mu_B \sum_{\mathbf{q}} \left\{1 - \frac{A(\mathbf{q})}{\hbar\ \omega_D(\mathbf{q})}\right\} \tag{7.405}$$

We can split the magnetization into an isotropic and an anisotropic part

$$M(T, B_0) = M_i(T, B_0) + M_a(T, B_0) \tag{7.406}$$

M_i is the magnetization of the isotropic ferromagnet:

$$M_i(T, B_0) = M_0 \left(1 - \frac{1}{NS}\sum_{\mathbf{q}} \langle n_{\mathbf{q}}\rangle\right) \tag{7.407}$$

M_0 denotes the magnetization of the fully ordered spin system

$$M_0 = g_J\ \mu_B\ \frac{N}{V}\ S \tag{7.408}$$