3.4 Linear response of the Heisenberg ferromagnet

In this section, we shall illustrate the use of linear response theory by applying it to the case of the three-dimensional Heisenberg ferromagnet, with the Hamiltonian

$$\mathcal{H} = -\frac{1}{2} \sum_{i \neq j} \mathcal{J}(ij)\, \mathbf{S}_i \cdot \mathbf{S}_j, \qquad (3.4.1)$$

where $\mathbf{S}_i$ is the spin on the ith ion, placed in a Bravais lattice at the position $\mathbf{R}_i$. The spatial Fourier transform of the exchange coupling, with the condition $\mathcal{J}(ii) \equiv 0$, is

$$\mathcal{J}(\mathbf{q}) = \frac{1}{N} \sum_{ij} \mathcal{J}(ij)\, e^{-i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)} = \sum_{j} \mathcal{J}(ij)\, e^{-i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)}, \quad (3.4.2a)$$

and conversely

$$\mathcal{J}(ij) = \frac{1}{N} \sum_{\mathbf{q}} \mathcal{J}(\mathbf{q})\, e^{i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)} = \frac{V}{N(2\pi)^3} \int \mathcal{J}(\mathbf{q})\, e^{i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)} d\mathbf{q},$$
$$(3.4.2b)$$

depending on whether $\mathbf{q}$, defined within the primitive Brillouin zone, is considered to be a discrete or a continuous variable (we shall normally assume it to be discrete). N is the total number of spins, V is the volume, and the inversion symmetry of the Bravais lattice implies that $\mathcal{J}(\mathbf{q}) = \mathcal{J}(-\mathbf{q}) = \mathcal{J}^*(\mathbf{q})$. The maximum value of $\mathcal{J}(\mathbf{q})$ is assumed to be $\mathcal{J}(\mathbf{q} = \mathbf{0})$, in which case the equilibrium state at zero temperature, i.e. the ground state, is the ferromagnet:

$$\langle \mathbf{S}_i \rangle = S\,\hat{\mathbf{z}} \qquad \text{at} \quad T = 0, \qquad (3.4.3)$$

where $\hat{\mathbf{z}}$ is a unit vector along the z-axis, which is established as the direction of magnetization by an infinitesimal magnetic field. This result is exact, but as soon as the temperature is increased above zero, it is necessary to make a number of approximations. As a first step, we

introduce the thermal expectation-values $\langle \mathbf{S}_i \rangle = \langle \mathbf{S} \rangle$ in the Hamiltonian which, after a simple rearrangement of terms, can be written

$$\mathcal{H} = \sum_i \mathcal{H}_i - \frac{1}{2} \sum_{i \neq j} \mathcal{J}(ij)(\mathbf{S}_i - \langle \mathbf{S} \rangle) \cdot (\mathbf{S}_j - \langle \mathbf{S} \rangle), \qquad (3.4.4a)$$

with

$$\mathcal{H}_i = -S_i^z \, \mathcal{J}(\mathbf{0}) \langle S^z \rangle + \tfrac{1}{2} \mathcal{J}(\mathbf{0}) \langle S^z \rangle^2, \qquad (3.4.4b)$$

and $\langle \mathbf{S} \rangle = \langle S^z \rangle \, \hat{\mathbf{z}}$. In the mean-field approximation, discussed in the previous chapter, the dynamic correlation between spins on different sites is neglected. This means that the second term in $(3.4.4a)$ is disregarded, reducing the original many-spin Hamiltonian to a sum of N independent single-spin Hamiltonians $(3.4.4b)$. In this approximation, $\langle S^z \rangle$ is determined by the self-consistent equation

$$\langle S^z \rangle = \sum_{M=-S}^{+S} M \, e^{\beta M \mathcal{J}(\mathbf{0}) \langle S^z \rangle} \Big/ \sum_{M=-S}^{+S} e^{\beta M \mathcal{J}(\mathbf{0}) \langle S^z \rangle} \qquad (3.4.5a)$$

(the last term in $(3.4.4b)$ does not influence the thermal average) which, in the limit of low temperatures, is

$$\langle S^z \rangle \simeq S - e^{-\beta S \mathcal{J}(\mathbf{0})}. \qquad (3.4.5b)$$

In order to incorporate the influence of two-site correlations, to leading order, we consider the Green function

$$G^{\pm}(ii', t) = \langle\langle S_i^+(t) \,;\, S_{i'}^- \rangle\rangle. \qquad (3.4.6)$$

According to $(3.3.14a)$, the variation in time of $G^{\pm}(ii', t)$ depends on the operator

$$[\, S_i^+ \,,\, \mathcal{H} \,] = -\frac{1}{2} \sum_j \mathcal{J}(ij) \left(-2S_i^+ S_j^z + 2S_i^z S_j^+ \right).$$

The introduction of this commutator in the equation of motion $(3.3.14a)$ leads to a relation between the original Green function and a new, more elaborate Green function. Through its equation of motion, this new function may be expressed in terms of yet another. The power of the exchange coupling in the Green functions which are generated in this way is raised by one in each step, and this procedure leads to an infinite hierarchy of coupled functions. An approximate solution may be obtained by utilizing the condition that the expectation value of S_i^z is close to its saturation value at low temperatures. Thus, in this limit,

S_i^z must be nearly independent of time, i.e. $S_i^z \simeq \langle S^z \rangle$. In this *random-phase approximation* (RPA) the commutator reduces to

$$[\, S_i^+ \,,\, \mathcal{H}\,] \simeq - \sum_j \mathcal{J}(ij)\langle S^z \rangle \left(S_j^+ - S_i^+ \right),$$

and the equations of motion lead to the following linear set of equations:

$$\hbar \omega G^{\pm}(ii', \omega) + \sum_j \mathcal{J}(ij)\langle S^z \rangle \left\{ G^{\pm}(ji', \omega) - G^{\pm}(ii', \omega) \right\}$$
$$= \langle\, [\, S_i^+ \,,\, S_{i'}^- \,]\, \rangle = 2 \langle S^z \rangle\, \delta_{ii'}. \tag{3.4.7}$$

The infinite set of RPA equations is diagonal in reciprocal space. Introducing the Fourier transform

$$G^{\pm}(\mathbf{q}, \omega) = \sum_{i'} G^{\pm}(ii', \omega)\, e^{-i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_{i'})}, \tag{3.4.8}$$

we obtain

$$\hbar \omega G^{\pm}(\mathbf{q}, \omega) + \langle S^z \rangle \left\{ \mathcal{J}(\mathbf{q}) G^{\pm}(\mathbf{q}, \omega) - \mathcal{J}(\mathbf{0}) G^{\pm}(\mathbf{q}, \omega) \right\} = 2 \langle S^z \rangle,$$

or

$$G^{\pm}(\mathbf{q}, \omega) = \lim_{\epsilon \to 0^+} \frac{2 \langle S^z \rangle}{\hbar \omega + i\hbar\epsilon - E_{\mathbf{q}}}, \tag{3.4.9}$$

where the *dispersion relation* is

$$E_{\mathbf{q}} = \langle S^z \rangle \left\{ \mathcal{J}(\mathbf{0}) - \mathcal{J}(\mathbf{q}) \right\}. \tag{3.4.10}$$

Introducing the susceptibility $\chi_{+-}(\mathbf{q}, \omega) = -G^{\pm}(\mathbf{q}, \omega)$, we obtain

$$\chi_{+-}(\mathbf{q}, \omega) = \frac{2 \langle S^z \rangle}{E_{\mathbf{q}} - \hbar \omega} + i\pi\, 2\langle S^z \rangle\, \delta(\hbar\omega - E_{\mathbf{q}}). \tag{3.4.11a}$$

Defining $\chi_{-+}(\mathbf{q}, \omega)$ analogously to $\chi_{+-}(\mathbf{q}, \omega)$, but with S^+ and S^- interchanged, we obtain similarly, or by the use of the symmetry relation (3.2.15),

$$\chi_{-+}(\mathbf{q}, \omega) = \frac{2 \langle S^z \rangle}{E_{\mathbf{q}} + \hbar \omega} - i\pi\, 2\langle S^z \rangle\, \delta(\hbar\omega + E_{\mathbf{q}}), \tag{3.4.11b}$$

so that the absorptive susceptibility is

$$\chi_{+-}''(\mathbf{q}, \omega) = -\chi_{-+}''(\mathbf{q}, -\omega) = 2\pi\, \langle S^z \rangle\, \delta(\hbar\omega - E_{\mathbf{q}}). \tag{3.4.11c}$$

The above susceptibilities do not correspond directly to physical observables but, for instance, $\chi_{xx}(\mathbf{q}, \omega)$ (where S^+ and S^- are both replaced by S_x) does. It is straightforward to see (by symmetry or by direct verification) that $\chi_{++}(\mathbf{q}, \omega) = \chi_{--}(\mathbf{q}, \omega) \equiv 0$, and hence

$$\chi_{xx}(\mathbf{q}, \omega) = \chi_{yy}(\mathbf{q}, \omega) = \tfrac{1}{4}\big\{\chi_{+-}(\mathbf{q}, \omega) + \chi_{-+}(\mathbf{q}, \omega)\big\}.$$

The presence of two-site correlations influences the thermal average $\langle S^z \rangle$. A determination of the correction to the MF result (3.4.5b) for $\langle S^z \rangle$, leading to a *self-consistent RPA* result for the transverse susceptibility, requires a relation between $\langle S^z \rangle$ and the susceptibility functions deduced above. The spin commutator-relation, $[\, S_i^+, \, S_{i'}^- \,] = 2S^z \delta_{ii'}$, turns out to be satisfied identically, and thus leads to no additional conditions. Instead we consider the *Wortis expansion*

$$S_i^z = S - \frac{1}{2S}S_i^- S_i^+ - \frac{1}{8S^2(S - \frac{1}{2})}(S_i^-)^2(S_i^+)^2 - \cdots \qquad (3.4.12)$$

for which the matrix elements between the p lowest single-spin (or MF) levels are correct, where $p \leq 2S + 1$ is the number of terms in the expansion. Using (3.4.11), we find from the fluctuation–dissipation theorem (3.2.18):

$$\langle S_i^- S_i^+ \rangle = \frac{1}{N}\sum_{\mathbf{q}} S_{-+}(\mathbf{q}, t = 0)$$

$$= \frac{1}{N}\sum_{\mathbf{q}} \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{1}{1 - e^{-\beta\hbar\omega}}\chi_{-+}''(\mathbf{q}, \omega)d(\hbar\omega) = 2\langle S^z \rangle\, \Phi,$$

$$(3.4.13a)$$

with

$$\Phi = \frac{1}{N}\sum_{\mathbf{q}} n_{\mathbf{q}} \qquad ; \qquad n_{\mathbf{q}} = \frac{1}{e^{\beta E_{\mathbf{q}}} - 1}, \qquad (3.4.13b)$$

where $n_{\mathbf{q}}$ is the population factor for bosons of energy $E_{\mathbf{q}}$. If $S = \frac{1}{2}$, then S^z is determined by the two first terms of (3.4.12), and

$$\langle S^z \rangle = S - \Phi\langle S^z \rangle/S,$$

or

$$\langle S^z \rangle = S^2/(S + \Phi) \simeq \tfrac{1}{2} - \Phi + 2\Phi^2 - \cdots$$

In general one may use a 'Hartree–Fock decoupling', $\langle (S_i^-)^2(S_i^+)^2 \rangle \simeq 2(\langle S_i^- S_i^+ \rangle)^2$, of the higher-order terms in (3.4.13) in order to show that

$$\langle S^z \rangle = S - \Phi + (2S + 1)\Phi^{2S+1} - \cdots \simeq S - \frac{1}{N}\sum_{\mathbf{q}} n_{\mathbf{q}}, \qquad (3.4.14)$$

where the *kinematic correction*, of the order Φ^{2S+1}, due to the limited number of single-spin states, which is neglected in this expression, is unimportant when $S \geq 1$. Utilizing the Hartree–Fock decoupling once more to write $\langle S_i^z S_j^z \rangle_{(i \neq j)} \simeq \langle S^z \rangle^2 \simeq S^2 - 2\langle S^z \rangle \Phi$, we find the internal energy to be

$$
\begin{aligned}
U = \langle \mathcal{H} \rangle &= -\tfrac{1}{2} N \mathcal{J}(\mathbf{0}) S^2 + \sum_{\mathbf{q}} E_{\mathbf{q}} \, n_{\mathbf{q}} \\
&= -\tfrac{1}{2} N \mathcal{J}(\mathbf{0}) S(S+1) + \sum_{\mathbf{q}} E_{\mathbf{q}} (n_{\mathbf{q}} + \tfrac{1}{2}).
\end{aligned}
\tag{3.4.15}
$$

The second form, expressing the effect of the zero-point motion, is derived using $\mathcal{J}(ii) = \frac{1}{N} \sum_{\mathbf{q}} \mathcal{J}(\mathbf{q}) \equiv 0$.

The thermodynamic properties of the Heisenberg ferromagnet are determined by (3.4.10), (3.4.14), and (3.4.15), which are all valid at low temperatures. In a cubic crystal, the energy dispersion $E_{\mathbf{q}}$ is isotropic and proportional to q^2 in the long wavelength limit, and (3.4.14) then predicts that the magnetization $\langle S^z \rangle$ decreases from its saturation value as $T^{3/2}$. The specific heat is also found to be proportional to $T^{3/2}$. The thermodynamic quantities have a very different temperature dependence from the exponential behaviour (3.4.5b) found in the MF approximation. This is due to the presence of elementary excitations, which are easily excited thermally in the long wavelength limit, since $E_{\mathbf{q}} \to 0$ when $\mathbf{q} \to \mathbf{0}$ in the RPA. These normal modes, which are described as *spin waves*, behave in most aspects (disregarding the kinematic effects) as non-conserved Bose-particles, and they are therefore also called *magnons*.

We shall not present a detailed discussion of the low-temperature properties of the Heisenberg ferromagnet. Further details may be found in, for instance, Marshall and Lovesey (1971), and a quite complete treatment is given by Tahir-Kheli (1976). The RPA model is correct at $T = 0$ where $\langle S^z \rangle = S$, but as soon as the temperature is increased, the magnons start to interact with each other, giving rise to finite lifetimes, and the temperature dependence of the excitation energies is modified (or *renormalized*). The temperature dependence of $E_{\mathbf{q}} = E_{\mathbf{q}}(T)$ is responsible for the leading order 'dynamic' corrections to $\langle S^z \rangle$ and to the heat capacity. A more accurate calculation, which we will present in Section 5.2, adds an extra term to the dispersion:

$$
E_{\mathbf{q}} = \langle S^z \rangle \{ \mathcal{J}(\mathbf{0}) - \mathcal{J}(\mathbf{q}) \} + \frac{1}{N} \sum_{\mathbf{k}} \{ \mathcal{J}(\mathbf{k}) - \mathcal{J}(\mathbf{k} + \mathbf{q}) \} n_{\mathbf{k}}, \tag{3.4.16}
$$

from which the heat capacity of this non-interacting Bose-gas can be determined as

$$
C = \partial U / \partial T = \sum_{\mathbf{q}} E_{\mathbf{q}} \, dn_{\mathbf{q}} / dT. \tag{3.4.17}
$$

We note that there are corrections to U, given by (3.4.15), of second order in Φ. The low-temperature properties, as determined by (3.4.14), (3.4.16), and (3.4.17), agree with the systematic expansion performed by Dyson (1956), including the leading-order dynamical correction of fourth power in T (in the cubic case), except for a minor kinematic correction which is negligible for $S \geq 1$.