FIP10604 – Text 07 — Magnons

Having discussed the ground state of the Heisenberg model in Text 06, we now turn to its properties at low but finite temperatures.

We begin by rewriting the Hamiltonian without explicit restriction to nearest-neighbor interactions, and using the set of operators $\{S^z, S^\pm\}$.

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

In the second equality, we used the property $J_{ij} = J_{ji}$, which allows us to exchange the summation indices in one of the sums, and the fact that spin operators corresponding to different sites commute.

FM Heisenberg Model at low temperatures

We will first restrict our analysis to the FM case, for which we know that long-range order exists in the ground state. As we saw in Text 06, the ground-state vector $|F\rangle$ satisfies the relations $S_i^z|F\rangle = S|F\rangle$ and $S_i^+|F\rangle = 0$ for any site i in the lattice. The energy of this state is $E_0 = -NS^2 J(\mathbf{0})$, where $J(\mathbf{0})$ is the Fourier transform of J_{ij},

$$J(\mathbf{k}) = \sum_i J_{ij} \, e^{i\mathbf{k}.(\mathbf{R}_i - \mathbf{R}_j)} \ , \tag{2}$$

evaluated at $\mathbf{k} = \mathbf{0}$. Notice that the sum on the right-hand side, although only over i, is independent of j due to the translation invariance of the lattice. For the same reason, the sum could be over j instead of i.

We can easily check that the z component of the **total** spin is conserved. Therefore, all energy eigenstates are characterized by a particular eigenvalue of $S_{\text{tot}}^z = \sum_i S_i^z$. As the eigenvalues of S_i^z differ by multiples of the unity (remembering that we are using $\mathbf{S}$ instead of $\mathbf{S}/\hbar$), the same happens with S_{tot}^z. The ground-state eigenvalue is NS. Thus, the eigenvalue corresponding to the first excited state must be $NS - 1$.

Consider, first, a spin deviation **localized** at site l, which we can represent by

$$|l\rangle = \frac{1}{\sqrt{2S}} S_l^- |F\rangle \ , \tag{3}$$

where $1/\sqrt{2S}$ is a normalization factor (it is easy to show that $\langle l|l'\rangle = \delta_{ll'}$).

Using the spin-operator algebra, we find that

$$\mathcal{H}|l\rangle = E_0|l\rangle + 2S \left[J(\mathbf{0})|l\rangle - \sum_i J_{il}|i\rangle \right] \ . \tag{4}$$

Therefore, $|l\rangle$ **is not** an eigenstate of $\mathcal{H}$. Given that there are N equivalent states of this type (the deviation may be at any one of the N lattice sites) any linear combination of them also corresponds to the same eigenvalue. In order to have an energy eigenstate we should seek a linear combination possessing the translation symmetry of the Hamiltonian. This can be done by choosing states of the form

$$|\mathbf{k}\rangle = \frac{1}{\sqrt{N}} \sum_i \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}_i}|i\rangle \;, \tag{5}$$

where $\mathbf{k}$ is clearly a wave vector. As we know, the restriction to finite size (N sites) must involve periodic boundary conditions, under which the wave-vector components take the values $k_\alpha = 2m_\alpha\pi/N_\alpha$, where m_α is an integer, $\alpha\,(=1,2,3)$ indexes the primitive lattice vectors (or x, y, z for the simple-cubic lattice), and $N_1 N_2 N_3 = N$. Hence, there are N independent vectors $\mathbf{k}$ (belonging to the first Brillouin zone).

To check that $|\mathbf{k}\rangle$ is an energy eigenvector we just apply $\mathcal{H}$ to it, obtaining

$$\mathcal{H}|\mathbf{k}\rangle = [E_0 + \varepsilon(\mathbf{k})]|\mathbf{k}\rangle \;, \tag{6}$$

with

$$\varepsilon(\mathbf{k}) = 2S\left[J(\mathbf{0}) - J(\mathbf{k})\right] \;. \tag{7}$$

The state $|\mathbf{k}\rangle$ can be interpreted as a ***spin wave***, $\varepsilon(\mathbf{k})$ being the **excitation energy** associated to its presence, since it is added to the ground-state energy E_0.

By analogy with the description of lattice vibrations through the *phonon* concept, we are tempted to write the Hamiltonian in the form

$$\mathcal{H} = E_0 + \sum_{\mathbf{k}} \varepsilon(\mathbf{k})\, a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \;, \tag{8}$$

where $a_{\mathbf{k}}^\dagger$ and $a_{\mathbf{k}}$ would be creation and annihilation operators of a "particle", called *magnon*, which carries an energy quantum $\varepsilon(\mathbf{k})$.

Still in analogy with phonons, we would expect the magnons to be bosons, and the Hamiltonian (8) would describe a Bose gas. Is this representation correct? To answer this question we must check whether the magnon operators obey a bosonic algebra (commutation relations).

We can define a local version of the magnon operators using Eq. (5), which allows us to write

$$a_{\mathbf{k}}^\dagger = \frac{1}{\sqrt{N}} \sum_i \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}_i} a_i^\dagger \;. \tag{9}$$

Then, by Eq. (3) we should have

$$a_i^\dagger = \frac{1}{\sqrt{2S}} S_i^- \quad\Rightarrow\quad a_i = \frac{1}{\sqrt{2S}} S_i^+ \;. \tag{10}$$

Finally, we would like to identify the product $a_i^\dagger a_i$ with n_i, the number operator for spin deviations ate site i. Thus, we would have

$$S_i^z = S - a_i^\dagger a_i = S - n_i \ . \tag{11}$$

However, Eqs. (10–11) yield the commutation relation

$$[a_i, a_j^\dagger] = \frac{1}{2S}[S_i^+, S_j^-] = \delta_{ij}\frac{S_i^z}{S} = \delta_{ij}(1 - n_i/S) \ , \tag{12}$$

that **does not** reproduce the appropriate relation for boson operators.

Holstein-Primakoff transformation

Based on the previous discussion, we define a transformation that preserves Eq. (11) and enforces a bosonic algebra of magnon operators, changing relations (10) in order to be consistent with the spin algebra. The new relations are

$$
\begin{aligned}
S_i^z &= S - n_i \ , \\
S_i^+ &= \sqrt{2S} \left(1 - \frac{n_i}{2S}\right)^{1/2} a_i \ , \\
S_i^- &= \sqrt{2S}\, a_i^\dagger \left(1 - \frac{n_i}{2S}\right)^{1/2} \ .
\end{aligned}
\tag{13}
$$

One can check (**EXERCISE**) that the algebra of spin operators is preserved if $[a_i, a_j^\dagger] = \delta_{ij}$ instead of Eq. (12).

Using the above relationships (known as *Holstein-Primakoff transformation*), we can rewrite the Heisenberg Hamiltonian as

$$\mathcal{H} = -\sum_{ij} J_{ij} \left[(S - n_i)(S - n_j) + 2Sa_i^\dagger \left(1 - \frac{n_i}{2S}\right)^{1/2} \left(1 - \frac{n_j}{2S}\right)^{1/2} a_j \right] \ . \tag{14}$$

This Hamiltonian is **exactly** equivalent to the original one. Its drawback is the presence of nonlinear terms, i.e., products of any number of operators (expanding the square roots). We can separate the Hamiltonian as

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 \ , \tag{15}$$

where $\mathcal{H}_0$ is a *single-particle* Hamiltonian,

$$\mathcal{H}_0 = E_0 + 2S \left[J(\mathbf{0}) \sum_i n_i - \sum_{ij} J_{ij}\, a_i^\dagger a_j \right] \ , \tag{16}$$

and $\mathcal{H}_1$ contains the *interaction terms*,

$$\mathcal{H}_1 = 2S \sum_{ij} J_{ij} \left\{ a_i^\dagger \left[1 - \left(1 - \frac{n_i}{2S} \right)^{1/2} \left(1 - \frac{n_j}{2S} \right)^{1/2} \right] a_j - \frac{n_i n_j}{2S} \right\} . \tag{17}$$

Rewritten in wave-vector space, $\mathcal{H}_0$ has exactly the form (8), describing the excitations of a FM Heisenberg system as a magnon gas. Neglecting $\mathcal{H}_1$ amounts to neglecting terms with $n_i/2S$. Since the maximum number of spin deviations at a site is $2S$, this approximation is good if the **average** number of spin deviations per site is small. This is expected to happen at low temperatures, when the system is close to the ground state, implying that the number of magnons is small. We must quantify what we mean by *low temperatures*. Clearly, the number of spin deviations per site becomes large as we approach the critical temperature T_C, above which the average spin becomes zero. Thus, a given temperature T is **low** if $T \ll T_C$.

Magnon dispersion relation at low energy

Equation (7) for the magnon energies can be simplified in the low-energy limit, which is relevant at low temperatures. Since $\varepsilon(\mathbf{k}) \to 0$ when $k \to 0$, we can expand $J(\mathbf{k})$ around $\mathbf{k} = \mathbf{0}$. Consider, for example, a generalization of the simple cubic lattice to d dimensions. In the nearest-neighbor approximation we have

$$J(\mathbf{k}) = 2J \sum_{\alpha=1}^{d} \cos(k_\alpha a) , \tag{18}$$

where a is the lattice parameter. Expanding to second order in $\mathbf{k}$ components, we obtain

$$J(\mathbf{k}) \simeq J(\mathbf{0}) - 2J \frac{(ka)^2}{2} \tag{19}$$

and Eq. (7) leads to

$$\varepsilon(\mathbf{k}) \simeq (2JSa^2)k^2 \equiv \mathcal{D}k^2 , \tag{20}$$

where $\mathcal{D}$ is called the spin wave's *stiffness constant*. This quadratic dispersion relation may be used in all calculations involving the magnon gas at low temperatures.

Magnetization and specific heat at $T \to 0$

For simplicity, we will assume that the magnetization is just the expected value of the local spin. This corresponds to defining the magnetization as the average magnetic moment per lattice site, and associating the magnetic moment directly to the spin, leaving aside a factor $-g\mu_B$. With this, the ratio between the magnetization magnitude and its saturation value

is equal to the ratio between the average value of a spin component and its maximum value. We then have

$$\frac{M}{M_0} = \frac{\langle S_i^z \rangle}{S} = \frac{1}{S}\left(S - \langle n_i \rangle\right) = 1 - \frac{1}{NS}\sum_{\mathbf{k}} \langle n_{\mathbf{k}} \rangle \,. \tag{21}$$

The equilibrium average energy (ground-state energy plus internal energy of the magnon gas) is given by

$$E = E_0 + \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \langle n_{\mathbf{k}} \rangle \,, \tag{22}$$

and its derivative with respect to temperature gives the magnetic contribution to the specific heat. Thus we see that both the spontaneous magnetization and the specific heat at low temperatures depend on the average number of magnons. As the magnons are bosons, $\langle n_{\mathbf{k}} \rangle$ for a system in thermodynamic equilibrium at temperature T is given by the Bose-Einstein distribution

$$\langle n_{\mathbf{k}} \rangle = \frac{1}{e^{\varepsilon(\mathbf{k})/T} - 1} \,, \tag{23}$$

where we choose a system of units in which energy and temperature are equivalent, i.e., $k_B = 1$.

In the limit $T \to 0$, we may use Eq. (20) for $\varepsilon(\mathbf{k})$. The deviations $\Delta M \equiv M_0 - M$ and $\Delta E \equiv E - E_0$, when calculated in the thermodynamic limit, may be expressed as integrals:

$$
\begin{aligned}
\frac{\Delta M}{M_0} &= \int \frac{\mathrm{d}^d k}{(2\pi)^d} \frac{1}{e^{\mathcal{D}k^2/T} - 1} \,, \\
\frac{\Delta E}{N} &= \int \frac{\mathrm{d}^d k}{(2\pi)^d} \frac{\mathcal{D}k^2}{e^{\mathcal{D}k^2/T} - 1} \,.
\end{aligned}
\tag{24}
$$

In the above equations, the wave vector k is a dimensionless quantity, corresponding to the product ka, where a is the lattice parameter of the hypercubic primitive cell. This is equivalent to choosing $a = 1$, i.e., a defines the length unit.

Eqs. (24) have integrands that depend only on the magnitude of $\mathbf{k}$, so that the angular part contributes a constant factor. For $T \to 0$, the upper limit of integration in k may be extended to infinity because the integrand is exponentially reduced as k increases. So, we are left with integrals of type

$$I_m(d,T) = \int_0^\infty \mathrm{d}k \, \frac{k^{d-1+m}}{e^{\mathcal{D}k^2/T} - 1} = \frac{1}{2}\left(\frac{T}{\mathcal{D}}\right)^{(d+m)/2} \int_0^\infty \mathrm{d}\xi \, \frac{\xi^{(d+m-2)/2}}{e^\xi - 1} \,. \tag{25}$$

At $d = 3$, the integral in ξ converges for both $m = 0$ and $m = 2$, which determine ΔM and ΔE, respectively. Therefore,

$$\frac{\Delta M}{M_0} \sim \left(\frac{T}{\mathcal{D}}\right)^{3/2} \,, \qquad \frac{\Delta E}{N} \sim \left(\frac{T}{\mathcal{D}}\right)^{5/2} \,. \tag{26}$$

The last equality indicates that the magnetic specific heat behaves as

$$c_m \sim T^{3/2} \ . \tag{27}$$

In summary, studying the Heisenberg model at low temperatures through magnons shows that the magnetization decreases from its saturation value following a power law ($\sim T^{3/2}$). The same power law appears for the specific-heat growth (from its null value at $T = 0$). These results are **exact** in the limit $T \to 0$, at which the simplifying assumptions that were made become strictly correct. Unfortunately, one cannot use this same formalism to study how these physical quantities behave as T approaches T_C.

Effect of dimensionality

We can see that the integral on ξ that appears in Eq. (25) **diverges** for $m = 0$ when $d = 2$ or $d = 1$. This indicates the **absence of spontaneous magnetization** for $T \neq 0$ at these spatial dimensions. The divergence comes from the $k \to 0$ limit, characterizing an *infrared divergence.*

We see thus that the Heisenberg model does not have an ordered phase at finite temperature in $d = 2$. This is in contrast to what happens with the Ising model, which does have an ordered phase, as we will see in detail later on. The difference will become clearer in the analyses that follow.

Applied magnetic field

In the presence of a uniform magnetic field, we add a Zeeman term, $-H \sum_i S_i^z$, to the Hamiltonian. As $S_i^z = S - n_i$, we have contributions to the ground-state energy and to the magnon-gas energy. The latter, in the limit $k \to 0$, becomes

$$\varepsilon_H(k) = H + \mathcal{D}k^2 \ . \tag{28}$$

It is clear that the field introduces a **gap** in the magnon dispersion relation. This eliminates the infrared divergences, allowing for magnetic order at $T \neq 0$ in any dimension, and leading to exponential behavior of ΔM and c_m with temperature.

It should be noted that the existence of magnetic order **does not** mean that there is a *phase transition*. In the presence of magnetic field, the system evolves **continuously** to the state of saturated magnetization as the temperature decreases.

System with anisotropy

As we saw in Text 04, a local axial anisotropy appears in the Hamiltonian as a term of type $-K \sum_i (S_i^z)^2$ (we use K instead of D to avoid confusion with the stiffness constant

$\mathcal{D}$). Let us concentrate on the easy-axis case, $K > 0$. In the magnon-gas approximation, the anisotropy term reduces to $-NKS^2 + 2SK\sum_i n_i$. So, in addition to a change in the ground-state energy, there is a term equivalent to a **magnetic field**, the *anisotropy field* $H_A = 2SK$.

This effect, in a certain way, allows us to understand the difference mentioned earlier between Heisenberg and Ising models in $d = 2$, since the Ising model may be seen as an extremely anisotropic Heisenberg model. However, unlike an actual applied field, the anisotropy does not eliminate the phase transition at T_C because the equivalence with a magnetic field is only valid in the limit of low number of spin deviations.

Magnons in the AF Heisenberg model

In Text 06 we observed that the ground state of the AF Heisenberg model cannot be written in a definite form. For this reason, to utilize magnons in this case we use the Néel state as a **reference state**.

The system is divided into two sublattices: A, corresponding to spin *up*, and B, corresponding to spin *down*. The Néel state, $|N\rangle$, is characterized by

$$S_i^z |N\rangle = \begin{cases} S|N\rangle \,, & i \in A \\ -S|N\rangle \,, & i \in B \,. \end{cases} \tag{29}$$

Spin deviations are caused by S_i^- if $i \in A$ and S_i^+ if $i \in B$. Using the notation i for the sites of sublattice A and j for those of sublattice B, we can introduce local bosonic operators for each sublattice, in the linear approximation, by the following equalities:

$$\begin{aligned} S_i^z &= S - a_i^\dagger a_i = S - n_i^a \,, \\ S_j^z &= -S + b_j^\dagger b_j = -S + n_j^b \,, \\ S_i^+ &= \sqrt{2S}\, a_i \,, \\ S_j^+ &= \sqrt{2S}\, b_i^\dagger \,. \end{aligned} \tag{30}$$

The Hamiltonian can then be written as

$$\mathcal{H} = -2\sum_{\substack{i\in A \\ j\in B}} J_{ij}\left[(S - n_i^a)(-S + n_j^b) + S(a_i^\dagger b_j^\dagger + a_i b_j)\right] - K\left[\sum_{i\in A}(S - n_i^a)^2 + \sum_{j\in B}(-S + n_j^b)^2\right]. \tag{31}$$

Notice the factor 2 in the first term because the sums over sites are restricted to each sublattice.

Using the nearest-neighbor approximation (with $J < 0$), neglecting quadratic terms in the number of local spin deviations, and going to wave-vector space, we obtain

$$\mathcal{H} = \bar{E}_0 + \sum_{\mathbf{k}} \left\{ \varepsilon_0 \left(n_{\mathbf{k}}^a + n_{\mathbf{k}}^b\right) - 2SJ(\mathbf{k}) \left[a_{\mathbf{k}}^\dagger b_{\mathbf{k}}^\dagger + a_{\mathbf{k}} b_{\mathbf{k}}\right] \right\} \,, \tag{32}$$

where
$$\bar{E}_0 = -N(z|J| + K)S^2 \, , \qquad \varepsilon_0 = H_A + 2z|J|S \, , \qquad H_A = 2SK \, . \tag{33}$$

The sum in Eq. (32) is over N wave vectors, since the Brillouin zone has been reduced to half its original size.

The Hamiltonian (32) is not diagonal in magnon operators which reflects the fact that the number of spin deviations **per sublattice** is not conserved. However, the **total** number of spin deviations, as discussed earlier, is conserved. We must then **diagonalize** the Hamiltonian, constructing appropriate linear combinations of the operators associated with the sublattices.

We define

$$
\begin{aligned}
c_{1\mathbf{k}} &= u_{\mathbf{k}} a_{\mathbf{k}} - v_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} \, , & c_{2\mathbf{k}} &= u_{\mathbf{k}} b_{\mathbf{k}} - v_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} \, , \\
c_{1\mathbf{k}}^{\dagger} &= u_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} - v_{\mathbf{k}} b_{\mathbf{k}} \, , & c_{2\mathbf{k}}^{\dagger} &= u_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} - v_{\mathbf{k}} a_{\mathbf{k}} \, ,
\end{aligned}
\tag{34}
$$

where we choose **real** coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$. Notice that $c_{1\mathbf{k}}$ and $c_{2\mathbf{k}}^{\dagger}$ are operators of type S^+, while the other two are of type S^-.

Imposing that the new operators satisfy bosonic commutation relations, we obtain

$$u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1 \, , \tag{35}$$

which allows us to parametrize the coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ as

$$u_{\mathbf{k}} = \cosh\theta_{\mathbf{k}} \, , \qquad v_{\mathbf{k}} = \sinh\theta_{\mathbf{k}} \, . \tag{36}$$

Inverting the relations (34), we have

$$
\begin{aligned}
a_{\mathbf{k}} &= u_{\mathbf{k}} c_{1\mathbf{k}} + v_{\mathbf{k}} c_{2\mathbf{k}}^{\dagger} \, , & b_{\mathbf{k}} &= u_{\mathbf{k}} c_{2\mathbf{k}} + v_{\mathbf{k}} c_{1\mathbf{k}}^{\dagger} \, , \\
a_{\mathbf{k}}^{\dagger} &= u_{\mathbf{k}} c_{1\mathbf{k}}^{\dagger} + v_{\mathbf{k}} c_{2\mathbf{k}} \, , & b_{\mathbf{k}}^{\dagger} &= u_{\mathbf{k}} c_{2\mathbf{k}}^{\dagger} + v_{\mathbf{k}} c_{1\mathbf{k}} \, .
\end{aligned}
\tag{37}
$$

Substitution of these operators in the Hamiltonian (32) results in

$$
\begin{aligned}
\mathcal{H} = {} & \bar{E}_0 + \sum_{\mathbf{k}} \left\{ \varepsilon_0 \left[(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2)(n_{1\mathbf{k}} + n_{2\mathbf{k}}) + 2v_{\mathbf{k}}^2 + 2u_{\mathbf{k}} v_{\mathbf{k}} (c_{1\mathbf{k}}^{\dagger} c_{2\mathbf{k}}^{\dagger} + c_{1\mathbf{k}} c_{2\mathbf{k}}) \right] \right. \\
& \left. - 2SJ(\mathbf{k}) \left[2u_{\mathbf{k}} v_{\mathbf{k}} (n_{1\mathbf{k}} + n_{2\mathbf{k}} + 1) + (u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2)(c_{1\mathbf{k}}^{\dagger} c_{2\mathbf{k}}^{\dagger} + c_{1\mathbf{k}} c_{2\mathbf{k}}) \right] \right\} \, .
\end{aligned}
\tag{38}
$$

The condition that non-diagonal terms are null implies that

$$\varepsilon_0 u_{\mathbf{k}} v_{\mathbf{k}} - SJ(\mathbf{k})(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2) = 0 \, . \tag{39}$$

Dividing by u_k^2, and using the parametrization (36) we obtain that $\theta_{\mathbf{k}}$ is determined by

$$\tanh(2\theta_{\mathbf{k}}) = \frac{2SJ(\mathbf{k})}{\varepsilon_0} \, . \tag{40}$$

On the other hand, the diagonal part of the Hamiltonian (38) may be written as

$$\mathcal{H} = \bar{E}_0 - \frac{N}{2}\varepsilon_0 + \sum_{\mathbf{k}} \varepsilon(\mathbf{k})[n_{1\mathbf{k}} + n_{2\mathbf{k}} + 1] \ , \tag{41}$$

with

$$\varepsilon(\mathbf{k}) = \varepsilon_0(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2) - 4SJ(\mathbf{k})\,u_{\mathbf{k}}v_{\mathbf{k}} \ . \tag{42}$$

Eliminating the coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ through Eqs. (36) and (40), the Hamiltonian becomes a sum of a ground-state energy and a (two-species) magnon gas,

$$\mathcal{H} = E_0 + \sum_{\mathbf{k}} \varepsilon(\mathbf{k})[n_{1\mathbf{k}} + n_{2\mathbf{k}}] \ , \tag{43}$$

where

$$E_0 = \bar{E}_0 - \frac{N}{2}\varepsilon_0 + \sum_{\mathbf{k}} \varepsilon(\mathbf{k}) \tag{44}$$

and

$$\varepsilon(\mathbf{k}) = \sqrt{\varepsilon_0^2 - [2SJ(\mathbf{k})]^2} \ . \tag{45}$$

In the absence of anisotropy ($K = 0$), these quantities take a simpler form,

$$
\begin{aligned}
E_0 &= -Nz|J|S(S+1) + \sum_{\mathbf{k}} \varepsilon(\mathbf{k}) \ , \\
\varepsilon(\mathbf{k}) &= 2S\sqrt{(zJ)^2 - J^2(\mathbf{k})} = 2z|J|S\sqrt{1 - \gamma_{\mathbf{k}}^2} \ ,
\end{aligned}
\tag{46}
$$

where

$$\gamma_{\mathbf{k}} \equiv \frac{1}{z}\sum_{\boldsymbol{\delta}} e^{i\mathbf{k}\cdot\boldsymbol{\delta}} \ . \tag{47}$$

There are z vectors $\boldsymbol{\delta}$ connecting a site to its z neighbors. All these vectors have magnitude a (the lattice parameter) in a cubic lattice. Then, in the limit $k \to 0$, expanding $\gamma_{\mathbf{k}}$ up to order $(\mathbf{k}\cdot\boldsymbol{\delta})^2$, we obtain

$$\varepsilon(\mathbf{k}) \simeq (2\sqrt{2z}\,|J|Sa)\,k \ . \tag{48}$$

Therefore, unlike the FM case, in an antiferromagnet we have magnons with a **linear** dispersion relation. This is exactly what happens to phonons, allowing us to predict the same type of behavior for the low-temperature specific heat, i.e.,

$$c_m \sim T^3 \ . \tag{49}$$

Ground state energy

Equation (44) shows that there is a *zero-point* magnon contribution to the AF ground state. That equation may be rewritten in the form

$$E_0 = -Nz|J|S^2\left(1 + \frac{\lambda}{S}\right) ,\tag{50}$$

where we defined

$$\lambda = 1 - \frac{2}{N}\sum_{\mathbf{k}}\sqrt{1 - \gamma_{\mathbf{k}}^2} .\tag{51}$$

E_0 would coincide with the average energy of the Néel state (E_N) if we had $\lambda = 0$. A numerical calculation for the simple-cubic lattice results in $\lambda \sim 0.1$, showing that $E_0 < E_N$.

Sublattice magnetization at $T = 0$

We know that the Néel state is not the ground state (and not even an eigenstate) of the AF Heisenberg Hamiltonian. Therefore, the sublattice magnetization at $T = 0$ should not be saturated. This magnetization is given by

$$M_0 = \langle S_{iA}^z\rangle_0 = \frac{2}{N}\sum_{i\in A}(S - \langle n_i^a\rangle_0) ,\tag{52}$$

where $\langle...\rangle_0$ indicates that the average is taken on the ground state. Then

$$M_0 = S - \frac{2}{N}\sum_{\mathbf{k}}\langle n_{\mathbf{k}}^a\rangle_0 \equiv S - \Delta M_0 .\tag{53}$$

As $n_{\mathbf{k}}^a = a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$, using the transformations (37) we obtain

$$n_{\mathbf{k}}^a = u_{\mathbf{k}}^2 n_{1\mathbf{k}} + v_{\mathbf{k}}^2(n_{2\mathbf{k}} + 1) + u_{\mathbf{k}}v_{\mathbf{k}}(c_{1\mathbf{k}}^\dagger c_{2\mathbf{k}}^\dagger + c_{1\mathbf{k}}c_{2\mathbf{k}}) .\tag{54}$$

After taking the ground-state average (zero magnons), we are left with

$$\langle n_{\mathbf{k}}^a\rangle_0 = v_{\mathbf{k}}^2 = \sinh^2\theta_{\mathbf{k}} = \frac{1}{2}\left[\frac{\varepsilon_0}{\varepsilon(\mathbf{k})} - 1\right] .\tag{55}$$

Using $\varepsilon(\mathbf{k})$ from Eq. (46), and substituting in Eq. (53), we arrive at

$$\Delta M_0 = \frac{1}{N}\sum_{\mathbf{k}}\left[\frac{1}{\sqrt{1 - \gamma_{\mathbf{k}}^2}} - 1\right] .\tag{56}$$

Numerical calculations for the simple-cubic lattice indicate that $\Delta M_0/S \sim 10\%$.

On the other hand, for the **one-dimensional** case in the thermodynamic limit, choosing an arbitrary k_0, small but nonzero, Eq. (56) yields

$$\Delta M_0 \sim \int_0^{k_0} \frac{\mathrm{d}k}{k} + (\text{finite terms}) .\tag{57}$$

The integral diverges at the lower limit of integration (infrared divergence). Therefore, the AF Heisenberg model in $d = 1$ **does not** show long range order **even at** $T = 0$. This limit will be discussed in more detail in another Text.