Renormalized magnons in quantum Heisenberg model

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1 Correlation functions

1.1 Definition and basic properties

• for a Hamiltonian H, time variable t, and two operators A and B, the correlation function $\langle A(t)B\rangle$ is defined as

$$\langle A(t)B\rangle \;=\; Z^{-1}\,\mathrm{Tr}\,\{\exp(-\beta H)A(t)B\}\;, \tag{1}$$

where

$$Z \;=\; \mathrm{Tr}\,\{\exp(-\beta H)\}$$

is the partition function, $\beta = 1/(k_B T)$ and (with $\hbar = 1$)

$$A(t) \;=\; \exp(iHt)A\exp(-iHt)$$

is the time dependent operator A in the Heisenberg representation

• in the basis of eigenvectors $|m\rangle$ of the Hamiltonian H with eigenvalues E_m and with matrix elements denoted as $\langle m|A|n\rangle = A_{mn}$ and $\langle m|B|n\rangle = B_{mn}$, an explicit expression for the correlation function is

$$\langle A(t)B\rangle \;=\; Z^{-1}\sum_{mn} A_{mn}B_{nm}\exp(-iE_nt)\exp(-\beta E_m)\exp(iE_mt)\,. \tag{2}$$

Similar expressions hold for a related correlation function $\langle BA(t)\rangle$:

$$\begin{aligned}\langle BA(t)\rangle \;&=\; Z^{-1}\,\mathrm{Tr}\,\{\exp(-\beta H)BA(t)\}\\ &=\; Z^{-1}\sum_{mn} A_{mn}B_{nm}\exp(iE_mt)\exp(-\beta E_n)\exp(-iE_nt)\,. \end{aligned}\tag{3}$$

• the Fourier transformations between the time (t) and frequency (ω) variables are defined as

$$\tilde{f}(\omega) \;=\; \int_{-\infty}^{\infty} \exp(i\omega t) f(t) \mathrm{d}t \,, \qquad f(t) \;=\; \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(-i\omega t) \tilde{f}(\omega) \mathrm{d}\omega \tag{4}$$

• using the well-known representation of the Dirac δ-function, namely

$$\int_{-\infty}^{\infty} \exp(i\omega t) \mathrm{d}t \;=\; 2\pi\, \delta(\omega) \,,$$

the Fourier transforms of the correlation functions $\langle A(t)B\rangle$ and $\langle BA(t)\rangle$ are equal to

$$\begin{aligned} \langle A(.)B\rangle(\omega) &\equiv \int_{-\infty}^{\infty} \exp(i\omega t) \langle A(t)B\rangle \mathrm{d}t \\ &= 2\pi Z^{-1} \sum_{mn} A_{mn} B_{nm} \exp(-\beta E_m)\, \delta(\omega + E_m - E_n) \,, \\ \langle BA(.)\rangle(\omega) &\equiv \int_{-\infty}^{\infty} \exp(i\omega t) \langle BA(t)\rangle \mathrm{d}t \\ &= 2\pi Z^{-1} \sum_{mn} A_{mn} B_{nm} \exp(-\beta E_n)\, \delta(\omega + E_m - E_n) \,. \end{aligned} \tag{5}$$

By employing an identity

$$\exp(-\beta E_n)\, \delta(\omega + E_m - E_n) \;=\; \exp(-\beta\omega) \exp(-\beta E_m)\, \delta(\omega + E_m - E_n) \,,$$

one can prove a general relation between the Fourier transforms in Eq. (5):

$$\langle BA(.)\rangle(\omega) \;=\; \exp(-\beta\omega)\, \langle A(.)B\rangle(\omega) \,. \tag{6}$$

Inverse relations to Eq. (5) are:

$$\begin{aligned} \langle A(t)B\rangle &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(-i\omega t)\, \langle A(.)B\rangle(\omega)\, \mathrm{d}\omega \,, \\ \langle BA(t)\rangle &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(-i\omega t)\, \langle A(.)B\rangle(\omega)\; \exp(-\beta\omega)\, \mathrm{d}\omega \,. \end{aligned} \tag{7}$$

• *Example:* for a linear harmonic oscillator with frequency Ω, the Hamiltonian is

$$H \;=\; \Omega \left(a^{+}a + \frac{1}{2} \right) \,, \tag{8}$$

where a^{+} and a are creation and annihilation operators, and we get directly from Eq. (5) (and from the known spectrum of the Hamiltonian H):

$$\begin{aligned} \langle a^{+}(.)a\rangle(\omega) &= 2\pi \, \frac{1}{\exp(\beta\Omega) - 1}\, \delta(\omega + \Omega) \,, \\ \langle a(.)a^{+}\rangle(\omega) &= 2\pi \left[1 + \frac{1}{\exp(\beta\Omega) - 1} \right] \delta(\omega - \Omega) \,. \end{aligned} \tag{9}$$

Note that the oscillator frequency Ω ($\equiv$ system dynamics) is contained in the shifts of arguments of the two δ-functions while the two weights contain the Bose-Einstein occupation function $[\exp(\beta\Omega)-1]^{-1}$ ($\equiv$ statistics). The application of Eq. (7) for $t = 0$ leads to the well-known thermodynamic average

$$\langle a^+ a\rangle \;=\; \frac{1}{\exp(\beta\Omega)-1}\,. \tag{10}$$

1.2 Method of equations of motion

• time evolution of the operator $A(t)$

$$\frac{\mathrm{d}}{\mathrm{d}t}A(t) \;=\; -i[A(t),H]$$

leads to the equation of motion for the correlation function

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A(t)B\rangle \;=\; -i\langle[A(t),H]B\rangle \tag{11}$$

• the equation of motion is usually applied to a set of correlation functions; the higher correlation functions appearing on the r.h.s. of Eq. (11) have to be approximated by means of the original correlation functions in order to get a closed set of equations

• the time derivative in Eq. (11) can be removed by employing the frequency-dependent quantities $\langle A(.)B\rangle(\omega)$ and a trivial consequence of the Fourier transformation, Eq. (4), for the functions $f(t)$ and $\tilde{f}(\omega)$:

$$-i\omega\tilde{f}(\omega) \;=\; \int_{-\infty}^{\infty}\exp(i\omega t)\,\frac{\mathrm{d}f(t)}{\mathrm{d}t}\,\mathrm{d}t\,.$$

This leads to:

$$\omega\,\langle A(.)B\rangle(\omega) \;=\; \langle[A(.),H]B\rangle(\omega)\,. \tag{12}$$

• *Application:* for the linear harmonic oscillator, Eq. (8), the usual commutation rules

$$[a,a^+] \;=\; 1 \qquad\Longrightarrow\qquad [a^+,H] \;=\; -\Omega a^+ \tag{13}$$

yield for the correlation function $\langle a^+(.)a\rangle(\omega)$ a simple result [see Eq. (9)]:

$$(\omega+\Omega)\,\langle a^+(.)a\rangle(\omega) \;=\; 0 \qquad\Longrightarrow\qquad \langle a^+(.)a\rangle(\omega) \;=\; 2\pi\,w\,\delta(\omega+\Omega)\,,$$

where w is an unknown weight. Substitution of this result in Eq. (7) for $t = 0$ gives averages

$$\langle a^+ a \rangle \;=\; w\,, \qquad \langle a a^+ \rangle \;=\; w\,\exp(\beta\Omega)\,.$$

This can be combined with the thermodynamic average of Eq. (13),

$$\langle a a^+ \rangle - \langle a^+ a \rangle \;=\; 1 \qquad \Longrightarrow \qquad w\,[\exp(\beta\Omega) - 1] \;=\; 1\,,$$

which defines the weight w in agreement with the previous result, Eq. (9). Note that this derivation of the correlation function, Eq. (9), and its consequence, Eq. (10), required neither any knowledge of the spectrum nor evaluation of the infinite summations contained, e.g., in Eq. (5).

2 Heisenberg Hamiltonian for spins $S = 1/2$

2.1 Properties of spin operators

- the Hamiltonian is defined as

$$H \;=\; -\frac{1}{2}\sum_{mn} J_{mn}\,\mathbf{s}_m\cdot\mathbf{s}_n \;-\; \sum_m b_m s_m^z\,, \tag{14}$$

where indices m, n denote lattice sites, the $\mathbf{s}_m \equiv (s_m^x, s_m^y, s_m^z)$ are spin operators (with spin quantum number $S = 1/2$) at the m-th lattice site, the exchange integrals J_{mn} describe a pair interaction of the local spins ($J_{mm} = 0$, $J_{mn} = J_{nm}$), and the quantities b_m denote local magnetic fields pointing along z-direction

- the spin operators $\mathbf{s}_m$ can be realized using the 2×2 Pauli matrices:

$$\begin{aligned} s_m^x &= \frac{1}{2}\sigma_m^x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_m\,, \\ s_m^y &= \frac{1}{2}\sigma_m^y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_m\,, \\ s_m^z &= \frac{1}{2}\sigma_m^z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_m\,, \end{aligned} \tag{15}$$

and the related operators $s_m^\pm$ by matrices:

$$s_m^+ \;\equiv\; s_m^x + i s_m^y \;=\; \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_m\,,$$

$$s_m^- \;\equiv\; s_m^x - i s_m^y \;=\; \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_m \tag{16}$$

• these operators satisfy following commutation rules:

$$\begin{aligned} [s_m^x, s_n^y] &= i\delta_{mn}\, s_m^z\,, & [s_m^-, s_n^z] &= \delta_{mn}\, s_m^-\,, \\ [s_m^y, s_n^z] &= i\delta_{mn}\, s_m^x\,, & [s_m^-, s_n^x] &= -\delta_{mn}\, s_m^z\,, \\ [s_m^z, s_n^x] &= i\delta_{mn}\, s_m^y\,, & [s_m^-, s_n^y] &= i\delta_{mn}\, s_m^z \end{aligned} \tag{17}$$

2.2 Correlation functions of spin operators

• time evolution of the spin operator s_j^- due to the Hamiltonian H, Eq. (14), follows from Eq. (17)

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} s_j^- \;=\; -i[s_j^-, H] \;&=\; i b_j s_j^- \,+\, i \sum_n J_{jn}\, (-s_j^z s_n^x + i s_j^z s_n^y + s_j^- s_n^z) \\ &=\; i b_j s_j^- \,+\, i \sum_n J_{jn}\, (s_n^z s_j^- - s_j^z s_n^-) \end{aligned}$$

• exact equations of motion for correlation functions $\left\langle s_j^-(t) s_r^+ \right\rangle$ are

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \left\langle s_j^-(t) s_r^+ \right\rangle \;&=\; i b_j \left\langle s_j^-(t) s_r^+ \right\rangle \\ &\quad + i \sum_n J_{jn} \left\{ \left\langle s_n^z(t) s_j^-(t) s_r^+ \right\rangle - \left\langle s_j^z(t) s_n^-(t) s_r^+ \right\rangle \right\} \end{aligned} \tag{18}$$

• approximate reduction of the higher correlation functions is obtained by a decoupling (for $n \neq j$):

$$\left\langle s_n^z(t) s_j^-(t) s_r^+ \right\rangle \;\approx\; \overline{s_n^z} \left\langle s_j^-(t) s_r^+ \right\rangle \,, \tag{19}$$

where $\overline{s_n^z} = \langle s_n^z \rangle$ is the thermodynamic average; the equations of motion, Eq. (18), together with Eq. (19) represent an infinite but closed set of equations. The decoupling, Eq. (19), is called a random-phase approximation (RPA), see, e.g., S. V. Tyablikov: Methods of Quantum Theory of Magnetism (Nauka, 1975). This approximation is exact for ferromagnets at zero temperature.

2.3 Solution for a ferromagnet

• in the case of a ferromagnet on a Bravais lattice, all lattice sites are equivalent,

$$b_m \;=\; b\,, \qquad \overline{s_m^z} \;=\; \overline{s^z}\,,$$

and Eq. (18) is thus approximated by

$$\frac{\mathrm{d}}{\mathrm{d}t} \left\langle s_j^-(t) s_r^+ \right\rangle \;=\; ib \left\langle s_j^-(t) s_r^+ \right\rangle \,+\, i\,\overline{s^z} \sum_n J_{jn} \left\{ \left\langle s_j^-(t) s_r^+ \right\rangle - \left\langle s_n^-(t) s_r^+ \right\rangle \right\}$$

• with an abbreviation

$$\mathcal{J} \;=\; \sum_n J_{mn} \;>\; 0\,,$$

the final equations of motion are given by

$$\frac{\mathrm{d}}{\mathrm{d}t} \left\langle s_j^-(t) s_r^+ \right\rangle \;=\; i\,(b + \mathcal{J}\,\overline{s^z}\,) \left\langle s_j^-(t) s_r^+ \right\rangle \,-\, i\,\overline{s^z} \sum_n J_{jn} \left\langle s_n^-(t) s_r^+ \right\rangle \tag{20}$$

• transformation of Eq. (20) to the frequency variable ω is based on a definition [see Eq. (5)]:

$$\mathcal{M}_{jr}(\omega) \;=\; \left\langle s_j^-(.) s_r^+ \right\rangle (\omega)\,. \tag{21}$$

The resulting equations for $\mathcal{M}_{jr}(\omega)$ are [see Eq. (12)]:

$$-\omega \mathcal{M}_{jr}(\omega) \;=\; (b + \mathcal{J}\,\overline{s^z}\,)\,\mathcal{M}_{jr}(\omega) \;-\; \overline{s^z} \sum_n J_{jn} \mathcal{M}_{nr}(\omega)\,. \tag{22}$$

• since the ferromagnet is translationally invariant, Eq. (22) can be simplified by introducing the lattice Fourier transformation:

$$\begin{aligned} \tilde{J}(\mathbf{k}) \;&=\; \sum_n \exp(i\mathbf{k}\cdot\mathbf{T}_n)\, J_{n0}\,, \\ \tilde{\mathcal{M}}(\mathbf{k},\omega) \;&=\; \sum_n \exp(i\mathbf{k}\cdot\mathbf{T}_n)\, \mathcal{M}_{n0}(\omega)\,, \end{aligned} \tag{23}$$

where $\mathbf{k}$ is a vector from the 1st Brillouin zone (BZ) of the lattice and $\mathbf{T}_n$ denotes the n-th translational vector (the vector of the n-th lattice site). This yields:

$$-\omega \tilde{\mathcal{M}}(\mathbf{k},\omega) \;=\; (b + \mathcal{J}\,\overline{s^z}\,)\,\tilde{\mathcal{M}}(\mathbf{k},\omega) \;-\; \overline{s^z}\,\tilde{J}(\mathbf{k})\tilde{\mathcal{M}}(\mathbf{k},\omega)\,. \tag{24}$$

• the last equation, Eq. (24), can be rewritten as

$$[\omega + E(\mathbf{k})]\,\tilde{\mathcal{M}}(\mathbf{k},\omega) \;=\; 0\,, \tag{25}$$

where

$$E(\mathbf{k}) \;=\; b \,+\, \overline{s^z} \left[\mathcal{J} - \tilde{J}(\mathbf{k}) \right] \tag{26}$$

denotes an excitation energy of the system—the magnon energy. The solution of Eq. (25) is given by

$$\tilde{\mathcal{M}}(\mathbf{k},\omega) \;=\; 2\pi\, w(\mathbf{k})\, \delta\Big(\omega + E(\mathbf{k})\Big)\,, \tag{27}$$

where $w(\mathbf{k})$ denotes an unknown weight. A comparison of Eq. (27) with the result for the linear harmonic oscillator, Eq. (9), and the lattice Fourier transformation, Eq. (23), suggest that the creation operator of the excitation—the magnon (or a spin wave)—with a given $\mathbf{k}$-vector is proportional to

$$a^+(\mathbf{k}) \sim \sum_n \exp(i\mathbf{k}\cdot\mathbf{T}_n)\, s_n^- \,. \tag{28}$$

2.4 Properties of single-magnon states

2.4.1 Ground state

• let us consider a state with all spins pointing up:

$$|0\rangle \;=\; \prod_n \otimes\, |\uparrow\rangle_n \,; \tag{29}$$

its elementary properties are:

$$s_n^z|0\rangle \;=\; \frac{1}{2}\,|0\rangle\,, \qquad s_n^+|0\rangle \;=\; 0\,, \tag{30}$$

and it can be shown that this state is an eigenstate of two operators, namely the z-component of the total spin

$$S^z \;=\; \sum_n s_n^z \tag{31}$$

and of the Hamiltonian H_0 without an external field [see Eq. (14)]

$$H_0 \;=\; -\,\frac{1}{2}\sum_{mn} J_{mn}\,\mathbf{s}_m\cdot\mathbf{s}_n \;=\; -\,\frac{1}{2}\sum_{mn} J_{mn}\,(s_m^- s_n^+ + s_m^z s_n^z)\,. \tag{32}$$

In particular,

$$S^z|0\rangle \;=\; \frac{N}{2}\,|0\rangle\,, \qquad H_0|0\rangle \;=\; -\,\frac{N\mathcal{J}}{8}\,|0\rangle\,, \tag{33}$$

where N is the number of sites (in a big finite crystal with periodic boundary conditions).

• for a ferromagnet, the state $|0\rangle$ is the ground state of the Hamiltonian H_0 but the corresponding eigenvalue $(-N\mathcal{J}/8)$ is infinitely degenerated; $|0\rangle$ is the non-degenerated ground state of the Hamiltonian H, Eq. (14), with a positive external field ($b_n = b > 0$)

2.4.2 Local spin flips

• states (normalized to unity) with a single spin pointing down are given by

$$|\lambda_n\rangle \;=\; s_n^-|0\rangle\,; \tag{34}$$

they are eigenstates of the total spin operator,

$$S^z|\lambda_n\rangle \;=\; \left(\frac{N}{2}-1\right)|\lambda_n\rangle\,, \tag{35}$$

but they are not eigenvectors of the Hamiltonian H_0

• the average value of H_0 in the state $|\lambda_n\rangle$ is given by

$$\langle\lambda_n|H_0|\lambda_n\rangle \;=\; -\,\frac{N\mathcal{J}}{8} + \frac{\mathcal{J}}{2}\,,$$

which means that the energy cost of a single-spin reversal is equal to $\mathcal{J}/2$

2.4.3 Single-magnon states

• let us define the creation operator of a magnon ($\mathbf{k} \in BZ$)

$$a^+(\mathbf{k}) \;=\; \frac{1}{\sqrt{N}}\sum_n \exp(i\mathbf{k}\cdot\mathbf{T}_n)\,s_n^-\,, \tag{36}$$

which differs from Eq. (28) only by the prefactor $N^{-1/2}$ (introduced for reasons of normalization); its action on the ground state, Eq. (29), yields a single-magnon state (normalized to unity)

$$\begin{aligned} |\mu(\mathbf{k})\rangle \;&=\; a^+(\mathbf{k})|0\rangle \;=\; \frac{1}{\sqrt{N}}\sum_n \exp(i\mathbf{k}\cdot\mathbf{T}_n)\,s_n^-|0\rangle \\ &=\; \frac{1}{\sqrt{N}}\sum_n \exp(i\mathbf{k}\cdot\mathbf{T}_n)\,|\lambda_n\rangle\,, \end{aligned} \tag{37}$$

so that the single-magnon state is a collective excitation, i.e., a linear combination of the local spin excitations $|\lambda_n\rangle$

• one can prove relations:

$$\left[S^z, a^+(\mathbf{k})\right] \;=\; -a^+(\mathbf{k})\,, \qquad S^z|\mu(\mathbf{k})\rangle \;=\; \left(\frac{N}{2}-1\right)|\mu(\mathbf{k})\rangle\,, \tag{38}$$

which show that the single-magnon state is an eigenstate of the total spin operator, Eq. (31), and that the excitation of one magnon reduces the total spin by unity, similarly to the local spin reversal [see Eq. (35)]

• one can also prove relations:

$$\begin{aligned}
\left[H_0, s_j^-\right] &= \sum_m J_{jm}(s_j^- s_m^z - s_m^- s_j^z)\,, \\
\left[H_0, s_j^-\right]|0\rangle &= \frac{\mathcal{J}}{2} s_j^- |0\rangle - \frac{1}{2}\sum_m J_{jm} s_m^- |0\rangle\,, \\
\left[H_0, a^+(\mathbf{k})\right]|0\rangle &= \frac{1}{2}\left[\mathcal{J} - \tilde{J}(\mathbf{k})\right] a^+(\mathbf{k})|0\rangle\,,
\end{aligned}$$

which yield

$$H_0|\mu(\mathbf{k})\rangle = \left[-\frac{N\mathcal{J}}{8} + E_0(\mathbf{k})\right]|\mu(\mathbf{k})\rangle\,, \tag{39}$$

with an abbreviation

$$E_0(\mathbf{k}) = \frac{1}{2}\left[\mathcal{J} - \tilde{J}(\mathbf{k})\right]\,. \tag{40}$$

This means that the single-magnon state is an eigenstate of the Hamiltonian, Eq. (32), and that the excitation of one magnon is connected with increase of energy by $E_0(\mathbf{k})$, Eq. (40), which is just the magnon energy $E(\mathbf{k})$, Eq. (26), in zero applied field ($b = 0$) and at zero temperature ($\overline{s^z} = 1/2$), see Fig. 1.

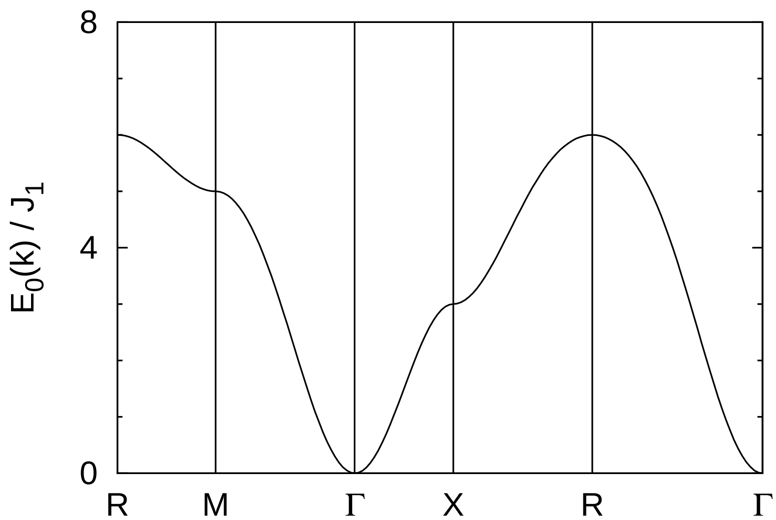

Figure 1: The magnon dispersion law, Eq. (40), for a ferromagnet on a simple cubic lattice with exchange interactions J_{mn} non-zero only between the first ($J_1 > 0$) and the second ($J_2 = J_1/8$) nearest neighbors. The magnon energy $E_0(\mathbf{k})$ is plotted along edges of the irreducible Brillouin zone of the simple cubic lattice.

• for long wavelengths, the magnon dispersion law $E_0(\mathbf{k})$ can be approximated by (see Fig. 1)

$$E_0(\mathbf{k}) \approx Dk^2 \qquad \text{for } |\mathbf{k}| \equiv k \to 0\,, \tag{41}$$

where D is the spin-wave stiffness constant. Excitation of such magnons is thus connected with a much smaller energy cost than that of a local spin reversal ($\mathcal{J}/2$), see section 2.4.2.

2.4.4 Two-magnon states

• the two-magnon states (unnormalized) can be defined similarly to the single-magnon states, Eq. (37):

$$\begin{aligned} |\mu^{(2)}(\mathbf{k}_1,\mathbf{k}_2)\rangle &= a^+(\mathbf{k}_1)a^+(\mathbf{k}_2)|0\rangle \\ &= \frac{1}{N}\sum_{mn} \exp(i\mathbf{k}_1\cdot\mathbf{T}_m)\exp(i\mathbf{k}_2\cdot\mathbf{T}_n)\, s_m^- s_n^-|0\rangle \end{aligned} \tag{42}$$

• one can prove relations analogous to Eq. (38):

$$\begin{aligned} \left[S^z, a^+(\mathbf{k}_1)a^+(\mathbf{k}_2)\right] &= -2a^+(\mathbf{k}_1)a^+(\mathbf{k}_2)\,, \\ S^z|\mu^{(2)}(\mathbf{k}_1,\mathbf{k}_2)\rangle &= \left(\frac{N}{2}-2\right)|\mu^{(2)}(\mathbf{k}_1,\mathbf{k}_2)\rangle\,, \end{aligned} \tag{43}$$

which show that the two-magnon state is an eigenstate of the total spin operator, Eq. (31), with the eigenvalue corresponding to a total spin reduction by two, i.e., the effects of the two magnons involved are strictly additive

• the two-magnon state is not an eigenstate of the Hamiltonian H_0; it can be proved that

$$\begin{aligned} \left[H_0, s_j^- s_r^-\right] &= s_j^- \sum_n J_{rn}(s_r^- s_n^z - s_n^- s_r^z) \,+\, s_r^- \sum_n J_{jn}(s_j^- s_n^z - s_n^- s_j^z) \\ &\quad + \delta_{jr} s_j^- \sum_n J_{jn} s_n^- \,-\, J_{jr} s_j^- s_r^-\,, \\ \left[H_0, s_j^- s_r^-\right]|0\rangle &= \frac{s_j^-}{2}\left(\mathcal{J}s_r^- - \sum_n J_{rn}s_n^-\right)|0\rangle \,+\, \frac{s_r^-}{2}\left(\mathcal{J}s_j^- - \sum_n J_{jn}s_n^-\right)|0\rangle \\ &\quad + \delta_{jr}s_j^-\left(\sum_n J_{jn}s_n^-\right)|0\rangle \,-\, J_{jr}s_j^- s_r^-|0\rangle\,. \end{aligned}$$

This relation has to be multiplied by $N^{-1}\exp(i\mathbf{k}_1\cdot\mathbf{T}_j)\exp(i\mathbf{k}_2\cdot\mathbf{T}_r)$ followed by summation over j and r, see Eq. (42), in order to get an expression for $[H_0, a^+(\mathbf{k}_1)a^+(\mathbf{k}_2)]|0\rangle$. The latter yields then a result:

$$\begin{aligned} H_0|\mu^{(2)}(\mathbf{k}_1,\mathbf{k}_2)\rangle &= \left[-\frac{N\mathcal{J}}{8} \,+\, E_0(\mathbf{k}_1) \,+\, E_0(\mathbf{k}_2)\right]|\mu^{(2)}(\mathbf{k}_1,\mathbf{k}_2)\rangle \\ &+ \frac{1}{N}\sum_{\mathbf{k}\in BZ}\tilde{J}(\mathbf{k})\left\{|\mu^{(2)}(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k},\mathbf{k})\rangle \,-\, |\mu^{(2)}(\mathbf{k}_1-\mathbf{k},\mathbf{k}_2+\mathbf{k})\rangle\right\}, \end{aligned} \tag{44}$$

where the first term corresponds to non-interacting excitations while the second term reflects the magnon-magnon interaction.

2.5 Selfconsistency condition

• the obtained relation for the correlation function, Eq. (27), does not represent the final solution to the problem since the weights $w(\mathbf{k})$ as well as the average value of the spin $\overline{s^z}$ and the magnon energies $E(\mathbf{k})$ have not been specified yet. In order to remove this ambiguity, one has to employ the algebra of the local spin operators, Eqs. (15, 16, 17).

• inverse lattice Fourier transformation to Eq. (23) yields

$$\mathcal{M}_{n0}(\omega) \;=\; \frac{1}{N} \sum_{\mathbf{k}\in BZ} \exp(-i\mathbf{k}\cdot\mathbf{T}_n)\, \tilde{\mathcal{M}}(\mathbf{k},\omega)\,, \tag{45}$$

where the number N of $\mathbf{k}$-points in the sum is equal to the number of sites in a big (but finite) crystal with periodic boundary conditions. Note that for $N \to \infty$, the sum in Eq. (45) is replaced by an integral over the BZ:

$$\lim_{N\to\infty} \frac{1}{N} \sum_{\mathbf{k}\in BZ} F(\mathbf{k}) \;=\; \frac{1}{V_{BZ}} \int_{BZ} F(\mathbf{k})\, \mathrm{d}^3\mathbf{k}\,,$$

where $F(\mathbf{k})$ is an arbitrary function and V_{BZ} denotes the volume of the BZ.

• inverse Fourier transformation with respect to time variable leads to [see Eq. (7)]:

$$\begin{aligned} \langle s_n^-(t) s_0^+ \rangle &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(-i\omega t) \mathcal{M}_{n0}(\omega) \mathrm{d}\omega\,, \\ \langle s_0^+ s_n^-(t) \rangle &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(-i\omega t) \mathcal{M}_{n0}(\omega) \exp(-\beta\omega) \mathrm{d}\omega \end{aligned}$$

• for the special case of $t = 0$, this reduces to

$$\begin{aligned} \langle s_n^- s_0^+ \rangle &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathcal{M}_{n0}(\omega) \mathrm{d}\omega\,, \\ \langle s_0^+ s_n^- \rangle &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathcal{M}_{n0}(\omega) \exp(-\beta\omega) \mathrm{d}\omega\,, \end{aligned}$$

and the use of Eq. (27) and Eq. (45) yields

$$\begin{aligned} \langle s_n^- s_0^+ \rangle &= \frac{1}{N} \sum_{\mathbf{k}\in BZ} \exp(-i\mathbf{k}\cdot\mathbf{T}_n)\, w(\mathbf{k})\,, \\ \langle s_0^+ s_n^- \rangle &= \frac{1}{N} \sum_{\mathbf{k}\in BZ} \exp(-i\mathbf{k}\cdot\mathbf{T}_n)\, w(\mathbf{k}) \exp[\beta E(\mathbf{k})] \end{aligned} \tag{46}$$

• let us employ a commutation relation that follows from Eq. (17),

$$[s_m^+, s_n^-] \;=\; 2\delta_{mn}\, s_m^z\,, \tag{47}$$

which yields after thermodynamic averaging

$$\langle [s_0^+, s_n^-] \rangle \;=\; \langle s_0^+ s_n^- \rangle - \langle s_n^- s_0^+ \rangle \;=\; 2\,\overline{s^z}\,\delta_{n0}\,,$$

and after substituting Eq. (46)

$$\frac{1}{N} \sum_{\mathbf{k}\in BZ} \exp(-i\mathbf{k}\cdot\mathbf{T}_n)\; \underbrace{w(\mathbf{k})\,\{\exp[\beta E(\mathbf{k})] - 1\}}_{g(\mathbf{k})} \;=\; 2\,\overline{s^z}\,\delta_{n0}\,.$$

This relation is valid for all lattice sites n (for all translation vectors $\mathbf{T}_n$) which implies that the function $g(\mathbf{k})$ reduces to a $\mathbf{k}$-independent constant, $g(\mathbf{k}) = 2\,\overline{s^z}$, and

$$w(\mathbf{k}) \;=\; \frac{2\,\overline{s^z}}{\exp[\beta E(\mathbf{k})] - 1}\,. \tag{48}$$

Note that the magnon weights $w(\mathbf{k})$ are proportional to the average spin $\overline{s^z}$ and to the Bose-Einstein occupation function for the magnon energies $E(\mathbf{k})$. The only unknown quantity in the weights $w(\mathbf{k})$, Eq. (48), and in the energies $E(\mathbf{k})$, Eq. (26), remains thus the average spin $\overline{s^z}$; for a given temperature T and external field b, the magnon weights and energies become renormalized according to the actual value of $\overline{s^z} = \overline{s^z}\,(T, b)$.

• one can further employ algebraic relations for spin operators on a single site, see Eq. (15):

$$s_n^+ s_n^- \;=\; \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}_n\,, \qquad s_n^- s_n^+ \;=\; \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}_n\,,$$

which yield

$$s_n^+ s_n^- + s_n^- s_n^+ \;=\; 1\,, \qquad s_n^z \;=\; \frac{1}{2} - s_n^- s_n^+\,. \tag{49}$$

The first of Eq. (49) gives after thermodynamic averaging

$$\langle s_0^+ s_0^- \rangle + \langle s_0^- s_0^+ \rangle \;=\; 1\,,$$

and after substituting Eq. (46) and Eq. (48)

$$\frac{1}{N} \sum_{\mathbf{k}\in BZ} w(\mathbf{k})\,\{\exp[\beta E(\mathbf{k})] + 1\} \;=\; 1\,,$$

$$2\,\overline{s^z}\,\frac{1}{N} \sum_{\mathbf{k}\in BZ} \frac{\exp[\beta E(\mathbf{k})] + 1}{\exp[\beta E(\mathbf{k})] - 1} \;=\; 2\,\overline{s^z}\,\frac{1}{N} \sum_{\mathbf{k}\in BZ} \coth\left[\frac{\beta E(\mathbf{k})}{2}\right] \;=\; 1\,.$$

• the latter equation together with Eq. (26) lead to a selfconsistency condition for $\overline{s^z}$:

$$\frac{1}{2\,\overline{s^z}} \;=\; \frac{1}{N} \sum_{\mathbf{k}\in BZ} \coth\left\{\frac{\beta\left\{b + \left[\mathcal{J} - \tilde{J}(\mathbf{k})\right]\overline{s^z}\right\}}{2}\right\}\,, \tag{50}$$

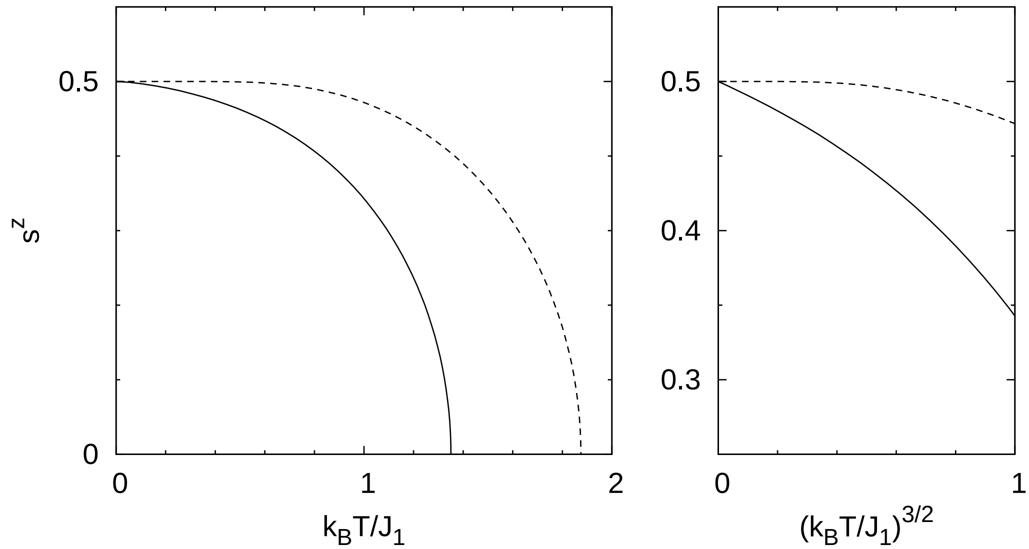

Figure 2: The temperature dependence of the spontaneous magnetization $\overline{s^z}$ as obtained from Eq. (50) for $b = 0$ and for the model defined in Fig. 1 (full lines). The dashed lines denote the dependence in the mean-field approximation; the right panel shows the low-temperature region and it illustrates the Bloch law, Eq. (55).

that closes the whole procedure and defines implicitly the dependence $\overline{s^z} = \overline{s^z}\,(T, b)$, see Fig. 2 for an example

2.6 Comparison to the MFA

• in the mean-field approximation (MFA) for the classical Ising model, the selfconsistency condition is:

$$\bar{s} \;=\; \tanh[\beta(b + \mathcal{J}\bar{s})]\,, \qquad \frac{1}{\bar{s}} \;=\; \coth[\beta(b + \mathcal{J}\bar{s})]\,,$$

while in the MFA for the quantum Heisenberg model, Eq. (14), it is given by:

$$2\,\overline{s^z} \;=\; \tanh\left[\frac{\beta(b + \mathcal{J}\,\overline{s^z}\,)}{2}\right]\,, \qquad \frac{1}{2\,\overline{s^z}} \;=\; \coth\left[\frac{\beta(b + \mathcal{J}\,\overline{s^z}\,)}{2}\right]\,.$$

These conditions are similar to Eq. (50), especially when a sum rule for the quantities $\tilde{J}(\mathbf{k})$,

$$\frac{1}{N}\sum_{\mathbf{k}\in BZ}\tilde{J}(\mathbf{k}) \;=\; J_{00} \;=\; 0\,, \tag{51}$$

is taken into account.

2.7 Curie temperature

• in the limit of small fields b and high temperatures T, $\coth(x) \approx x^{-1}$ for $|x| \ll 1$, and Eq. (50) reduces to

$$\frac{1}{2\,\overline{s^z}} = \frac{1}{N} \sum_{\mathbf{k}\in BZ} \frac{2}{\beta\left\{b + \left[\mathcal{J} - \tilde{J}(\mathbf{k})\right]\overline{s^z}\right\}} .$$

The Curie temperature is featured by existence of a small non-zero value of $\overline{s^z}$ in absence of external field ($b = 0$):

$$\frac{1}{2\,\overline{s^z}} = \frac{1}{N} \sum_{\mathbf{k}\in BZ} \frac{2}{\beta\left[\mathcal{J} - \tilde{J}(\mathbf{k})\right]\overline{s^z}} ,$$

which yields the following expression for the Curie temperature T_C^{RM}:

$$\frac{1}{k_B T_C^{RM}} = 4\,\frac{1}{N} \sum_{\mathbf{k}\in BZ} \frac{1}{\mathcal{J} - \tilde{J}(\mathbf{k})} . \qquad (52)$$

Note that for a ferromagnet, an inequality $\mathcal{J} \geq \tilde{J}(\mathbf{k})$ holds for all vectors $\mathbf{k} \in BZ$ [i.e., all magnon energies $E_0(\mathbf{k})$ are non-negative]

• the Curie temperature in the MFA, T_C^{MFA} is given explicitly by

$$k_B T_C^{MFA} = \frac{1}{4}\mathcal{J} = \frac{1}{4}\frac{1}{N} \sum_{\mathbf{k}\in BZ} \left[\mathcal{J} - \tilde{J}(\mathbf{k})\right] , \qquad (53)$$

where the second relation is valid due to Eq. (51). A comparison of the two Curie temperatures can be done using the well-known theorem on the arithmetic and harmonic averages of positive numbers; it results in

$$\frac{T_C^{MFA}}{T_C^{RM}} = \left\{\frac{1}{N} \sum_{\mathbf{k}\in BZ} \left[\mathcal{J} - \tilde{J}(\mathbf{k})\right]\right\} \left\{\frac{1}{N} \sum_{\mathbf{k}\in BZ} \frac{1}{\mathcal{J} - \tilde{J}(\mathbf{k})}\right\} > 1 ,$$

so that the renormalized magnons lead to a reduced Curie temperature as compared to the MFA (see Fig. 2).

2.8 Low-temperature behavior

• in the limit of low temperatures ($T \to 0$) and for an infinitesimal positive external field ($b \to 0^+$), the average magnetization tends to its saturated value $\overline{s^z} \to 1/2$. The deviation of $\overline{s^z}$ from this limiting value due to a small finite temperature $T > 0$ can be obtained from thermodynamic average of the second of Eq. (49):

$$\overline{s^z} = \frac{1}{2} - \langle s_0^- s_0^+ \rangle = \frac{1}{2} - \frac{1}{N} \sum_{\mathbf{k}\in BZ} w(\mathbf{k}) ,$$

where use has been made of Eq. (46). Substitution of Eq. (48) yields

$$\begin{aligned}\overline{s^z} &= \frac{1}{2} - \frac{1}{N}\sum_{\mathbf{k}\in BZ}\frac{2\,\overline{s^z}}{\exp[\beta E(\mathbf{k})]-1} \\ &\approx \frac{1}{2} - \frac{1}{N}\sum_{\mathbf{k}\in BZ}\frac{1}{\exp[\beta E_0(\mathbf{k})]-1}\,, \qquad (54)\end{aligned}$$

where we replaced the value of $\overline{s^z}$ at $T > 0$ by its zero-temperature limit in the latter expression and employed the magnon dispersion law at zero temperature, Eq. (40). The form of Eq. (54) shows that the initial reduction of the average magnetization is due to thermal excitation of magnons.

• the dominating contribution to the second term of Eq. (54) is due to low-energy magnons with long wavelength, see Eq. (41). For 3-dimensional systems, the second term in r.h.s. of Eq. (54) can be thus approximated by

$$\begin{aligned}\frac{1}{N}\sum_{\mathbf{k}\in BZ}\frac{1}{\exp[\beta E_0(\mathbf{k})]-1} &\approx \frac{1}{V_{BZ}}\int_{BZ}\frac{1}{\exp(\beta D k^2)-1}\,\mathrm{d}^3\mathbf{k} \\ \approx \frac{4\pi}{V_{BZ}}\int_0^\infty \frac{k^2}{\exp(\beta D k^2)-1}\,\mathrm{d}k &= \frac{2\pi}{V_{BZ}}\,(\beta D)^{-3/2}\int_0^\infty\frac{y^{1/2}}{\exp(y)-1}\,\mathrm{d}y\end{aligned}$$

so that finally

$$\overline{s^z}\,(T) \approx \frac{1}{2} - \alpha\, T^{3/2}\,, \qquad (55)$$

where α is a constant. Equation (55) is the Bloch's 3/2-law, see Fig. 2.

2.9 Renormalized magnons - a summary

• the theory of renormalized magnons for quantum isotropic Heisenberg ferromagnets is better than the MFA in following aspects:

+ it yields zero Curie temperature for 1- and 2-dimensional systems, in agreement with the Mermin-Wagner theorem

+ it reproduces the Bloch law for the low-temperature behavior of average magnetization in 3-dimensional systems

• the theory of renormalized magnons, however, fails in following points:

– the critical behavior is featured by critical exponents identical to those obtained within the MFA

– the magnetic short-range order above the Curie temperature is fully neglected, similarly to the MFA

– the finite lifetime of magnons (due to the magnon-magnon interaction) is neglected