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The Bosonic and Fermionic Green Functions in the Quantum Theory of Heisenberg Ferromagnet

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Abstract: The magnetization of ferromagnetic systems is treated within framework of many-body Green function theory by considering x- and z- components of the magnetization. We present a method for the calculation of expectation values in terms of the eigenvalues and eigenvectors of the equations of motion matrix for set of Green functions.

1. Introduction

The bosonic and fermionic Green functions theory of a Heisenberg model for the ferromagnet is presented. The bosonic Green function theory is appropriated when one considers an isotropic or unidirection system. In this case we need to calculate only one component of magnetization, i.e. the *z*-component. However, there exist cases where the system is anisotropic and not uniaxial. For example, under an external transversal magnetic field, the magnetization rotates with the variation of the field. In ferromagnetic ultra thin film, the magnetization may rotate with the variation of the temperature [1] and the film thickness [2]. The reorientation of magnetization in ferromagnetic thin films may be qualitatively understood by considerations of the competing shape and uniaxial anisotropy and was observed at the temperature below the Curie temperature in films of a few monolayers of Fe, Co, and Ni on Cu or Ag substrates. The orientation of the magnetization is determined by the components m_z, m_x. When one wants to calculate within Green function method more than one component of magnetization, the bosonic Green function theory is limited. The most serious problem encountered is that one of the dispersion relations (**q**)is always zero. The zero-frequency difficulties could be circumvented by means of the fermionic Green function [3–5].

2. The Theory

The time-dependent retarded Green function involving the two operators *A* and *B*, $A(t);B$, is defined by

$$G_{ij(\ )}(t) \quad A_i(t);B_j \quad i \ (t)\ [A_i(t),B_j] \quad , \qquad (1)$$

where subscripts i, j label sites in lattice, $A_i(t)$, is the spin operator at time t, B_j is the spin operator, (t) is the unity for positive t and zero for negative t, single angular brackets denote an average with respect to the canonical density matrix of the system at temperature T and

$$[A_i(t), B_j] \quad A_i(t)B_j \quad B_j A_i(t) , \qquad 1 . \tag{2}$$

In these equations the Green function is called the bosonic Green function, if $= -1$, or the fermionic Green function, if $= +1$. The equation of motion for $G_{ij(\ )}(t)$ is written as

$$i\frac{d}{dt}G_{ij(\ )}(t) \quad [A_i\ (t), B_j] \quad (t) \quad \langle\langle [A_i\ (t), H]; B_j \rangle\rangle \ . \tag{3}$$

Where (t) is the Dirac -function, brackets $[A_i\ (t), H]$ correspond to the commutator and $\hbar \quad 1$ has been used. The time Fourier transform of the Green function is a function of frequency , and is denoted by $G_{ij(\ )}(\ ) \quad A_i; B_j$. It satisfies the equation of motion

$$\langle\langle A_i; B_j \rangle\rangle \quad [A_i\ , B_j] \quad _{ij} \quad \langle\langle [A_i\ , H]\ ; B_j \rangle\rangle \ . \tag{4}$$

Where $_{ij}$ is the Kronecker symbol. For Heisenberg Hamiltonian H with general spin S, the operators A_i, B_j are taken as the following spin operators

$$A_i \quad S_i \text{ and } B_j \quad (S_j^z)^l (S_j\ )^m , \tag{5}$$

where l, m are zero or positive integers, necessary for dealing with higher spin values S.

Then the Green function is further Fourier transformed in real space

$$G_{ij(\ )}(\ ) \quad \frac{1}{N} \ _{\mathbf{q}} \ G_{\mathbf{q},\ }(\ )e^{i\mathbf{q}.(\mathbf{a}_i \ \ \mathbf{a}_j)}. \tag{6}$$

Here $\mathbf{q}$ is the wave vector and $\mathbf{a}_{i(j)}$ are the position vectors of the sites i, j. The integration over wave vector can be in one, two or three dimensions depending on the system studied. Now the Green function $G_{\mathbf{q}(\ )}(\ )$ is a function of wave vector $\mathbf{q}$ and frequency $= (\mathbf{q})$.

Statistical averages of the product of the two operators B_j and A_i (the correlation function $C_{ij} \quad B_j A_i$) is expressed in terms of the Green function by the spectral theorem

$$C_{ij} \quad B_j A_i \quad \lim_{0} \frac{1}{N} \ _{\mathbf{q}} \ e^{i\mathbf{q}.(\mathbf{a}_i \ \ \mathbf{a}_j)} \ \frac{i}{2} \ \frac{d}{e} (G_{\mathbf{q}(\ )}(\ \ i\ ) \ \ G_{\mathbf{q}(\ )}(\ \ i\ )) . \tag{7}$$

If the equation of motion can be solved for $G_{ij(\ )}(\ ) \quad A_i; B_j$ one then extracts knowledge of the correlation function $C_{ij} \quad B_j A_i$. Equations (4) and (7) are the only equations required for the application of the Green function method.

To solve the Green function, Hamiltonian H that appears in the equation of motion must be known. For simplicity, we only consider isotropic Hamiltonian

$$H \quad \frac{1}{2} \ _{i,j} \ J_{ij}\mathbf{S}_i.\mathbf{S}_j \quad \frac{1}{2} \ _{i,j} \ J_{ij}[S_i^z S_j^z \quad S_i\ S_j\ ], \tag{8}$$

where $J_{ij} - J > 0$ is the exchange integral corresponding to the interaction between the spins on lattice sites i, j. The notation $S_g \quad S_g^x \quad iS_g^y$ is introduced. Higher order Green function will appear in the equation of motion (4), too. It is to be decoupled by a random phase approximation (RPA). There are two decoupling procedures, namely asymmetric and symmetric decoupling.

2.1. Asymmetric decoupling

a) Bosonic Green functions

The exact equations of motion for Green functions are $G_{ij,}^{(\ ,l)}(\ ) \quad S_i \ ;(S_j^z)^l S_j$

$$\left\langle\left\langle S_i \ ;(S_j^z)^l S_j \right\rangle\right\rangle \quad [S_i \ ,(S_j^z)^l S_j \ ] \quad {}_{ij} \quad \left\langle\left\langle [S_i \ ,\mathcal{H}];(S_j^z)^l S_j \right\rangle\right\rangle \ . \tag{9}$$

The first term on the right side of (9) is given by

$$\left\langle [S_i \ ,(S_j^z)^l S_j \ ] \quad {}_1 \right\rangle \ {}_{ij} \quad A_{ij, \ \ 1}^{(\ ,l)} \ {}_{i,j}, \tag{10}$$

where

$$A_{i, \ \ 1}^{(\ ,l)} \quad 2\left\langle (S_i^z \quad 1)^l S_i^z \right\rangle \quad \left\langle \{(S_i^z \quad 1)^l \quad (S_i^z)^l\}\{S(S \quad 1) \quad S_i^z \quad (S_i^z)^2\}\right\rangle . \tag{11}$$

The commutator of S_i with the Hamiltonian *H*, required in the last term of (9), is easily computed, giving

$$[S_i \ ,\mathcal{H}] \quad \sum_{k \ i} J_{ik}(S_k^z S_i \quad S_i^z S_k \ ) . \tag{12}$$

The equations of motion (9) are then given by

$$S_i \ ;(S_j^z)^l S_j \quad {}^1 \quad A_{ij, \ \ 1}^{(\ ,l)} \ {}_{ij} \quad \sum_{k \ i} J_{ik}\{ \ S_k^z S_i \ ;(S_j^z)^l S_j \quad {}^1 \quad S_i^z S_k \ ;(S_j^z)^l S_j \quad {}^1\}. \tag{13}$$

The remaining problem is to express the higher order Green function on the right in terms of lower order Green functions, so that (13) can be explicitly solved for $G_{ij, \ \ 1}^{(\ ,l)}(\ ) \quad S_i \ ;(S_j^z)^l S_j \quad {}^1$. **Here asymmetric decoupling** means that

$$\left\langle\left\langle (S_k^z S_i \quad S_i^z S_k \ ;(S_j^z)^l S_j \right\rangle\right\rangle^1 \quad S^z \ (\ S_i \ ;(S_j^z)^l S_j \quad {}^1 \quad S_k \ ;(S_j^z)^l S_j \quad {}^1)$$
$$S^z \ (G_{ij, \ \ 1}^{(\ ,l)}(\ ) \quad G_{kj, \ \ 1}^{(\ ,l)}(\ )). \tag{14}$$

Inserting the decoupling approximation (14) into the equation of motion (13) gives

$$(\quad zJ \ S^z \ )G_{ij,, \ \ 1}^{(\ ,l)}(\ ) \quad A_{ij, \ \ 1}^{(\ ,l)} \ {}_{ij} \quad S^z \quad \sum_{k \ i} J_{ik} G_{kj, \ \ 1}^{(\ ,l)}(\ ) . \tag{15}$$

These equations are set of coupled equations for various pairs of sites (*i*,*j*), (*k*,*j*). Because of the translational invariance of the lattice we can transform the Fourier functions $G_{ij, \ \ 1}^{(\ ,l)}(\ )$, J_{ij} and ${}_{ij}$ with respect to the reciprocal lattice:

$$G_{ij, \ \ 1}^{(\ ,l)}(\ ) \quad \frac{1}{N} \sum_{\mathbf{q}} G_{\mathbf{q}, \ \ 1}^{(\ ,l)}(\ )e^{i\mathbf{q}.(\mathbf{a}_i \ \ \mathbf{a}_j)}, \ J_{ik} \quad \frac{1}{N} \sum_{\mathbf{q}} J(\mathbf{q})e^{i\mathbf{q}.(\mathbf{a}_i \ \ \mathbf{a}_k)}, \quad {}_{ij} \quad \frac{1}{N} \sum_{\mathbf{q}} e^{i\mathbf{q}.(\mathbf{a}_i \ \ \mathbf{a}_j)}. \tag{16}$$

where the parameter $J(\mathbf{q}) \quad J \quad e^{i\mathbf{q}.(\mathbf{a}_i \ \mathbf{a}_j)}$ and N is the number of the spins in the lattice. Equation (15) then implies $_j$

$$(\quad zJ \ S^z \ )G^{(\ ,l)}_{\mathbf{q}, \quad 1}(\ ) \quad A^{(\ ,l)}_{1} \quad S^z \ J(\mathbf{q})G^{(\ ,l)}_{\mathbf{q}, \quad 1}(\ ). \tag{17}$$

From (17) we get, $G^{(\ ,l)}_{\mathbf{q}, \quad 1}(\ )$, for the equation

$$G^{(\ ,l)}_{\mathbf{q}, \quad 1}(\ ) \quad \frac{A^{(\ ,l)}_{1}}{J(0) \quad S^z \quad (1 \quad J(\mathbf{q})/J(0))} \quad \frac{A^{(\ ,l)}_{1}}{\mathbf{q}}, \tag{18}$$

Where $J(0) \quad zJ, \quad _{\mathbf{q}} \quad J(0) \quad S^z \quad (1 \quad J(\mathbf{q})/J(0))$.
Between the Fourier transform $G^{(\ ,l)}_{\mathbf{q}}(\ )$ and the spectral function I_q exists the relation

$$I_{\mathbf{q}} \quad ^1(\ ) \quad \frac{i}{e \quad 1} \lim_{0} [G^{(\ ,l)}_{\mathbf{q}, \quad 1}(\quad i \ ) \quad G^{(\ ,l)}_{\mathbf{q}, \quad 1}(\quad i \ )]$$

$$\frac{iA^{(\ ,l)}_{1}}{e \quad 1} \lim_{0} \quad \frac{1}{_{\mathbf{q}} \quad i} \quad \frac{1}{_{\mathbf{q}} \quad i} \quad , \tag{19}$$

where the spectral function is connected with the correlation function by the relation

$$C^{(\ ,l)} \quad (S^z)^l S \ S \quad \frac{1}{2 \ N} \quad _{\mathbf{q}} \quad d \ \ I_{\mathbf{q}} \quad ^1(\ ). \tag{20}$$

Using the relation

$$\lim_{0} \quad d \quad \frac{f(\ )}{_{\mathbf{q}} \quad i} \quad P \ \ d \quad \frac{f(\ )}{_{\mathbf{q}}} \mp \ i \ \ d \ \ f(\ ) \ (\qquad _{\mathbf{q}}), \tag{21}$$

or its symbolic form

$$\lim_{0} \frac{f(\ )}{_{\mathbf{q}} \quad i} \quad P \ \frac{f(\ )}{_{\mathbf{q}}} \ \mp \ if(\ ) \ (\qquad _{\mathbf{q}}), \tag{21a}$$

the equation (19) can be written as

$$I_{\mathbf{q}} \quad ^1(\ ) \quad \frac{2 \ A^{(\ ,l)}_{1} \ (\qquad _{\mathbf{q}})}{e \quad 1}. \tag{22}$$

With the relation $[S^z, S \ ] \quad S$ and $S \ S \quad S(S \quad 1) \quad S^z \quad (S^z)^2$ we find that

$$(S^z)^l S \ S \qquad S(S \quad 1) \ (S^z)^l \quad (S^z)^{l \ 1} \quad (S^z)^{l \ 2} \ . \tag{23}$$

From (19) and (20) we get

$$(S^z)^l S \ S$$

$$\frac{1}{2 \ N} \quad _{\mathbf{q}} \quad d \ \ I_{\mathbf{q}} \quad ^1(\ ) \quad \frac{1}{2 \ N} \quad _{\mathbf{q}} \quad d \quad \frac{2 \ A^{(\ ,l)}_{1} \ (\qquad _{\mathbf{q}})}{e \quad 1} \quad \frac{A^{(\ ,l)}_{1}}{N} \quad _{\mathbf{q}} \ \frac{1}{e^{\ \mathbf{q}} \quad 1}. \tag{24}$$

If we use (11) and (23) we get

$$S(S \quad 1)\,(S^z)^l \quad (S^z)^{l\ 1} \quad (S^z)^{l\ 2} \tag{25}$$

$$(2\langle S_i^z \quad 1)^l S_i^z\rangle \quad \langle\{(S_i^z \quad 1)^l \quad (S_i^z)^l\}\{S(S \quad 1) \quad S_i^z \quad (S_i^z)^2\}\rangle)K\,,$$

where

$$K \quad \frac{1}{N}{}_{\mathbf{q}}\frac{1}{e^{\ \mathbf{q}} \quad 1}. \tag{26}$$

From (25) we can write down $2S$ independent, simultaneous linear equations in S^z , $(S^z)^2$,..., $(S^z)^{2S}$, by putting l in (24) equal 1, 2, … , 2S, consequently. Callen [6] shown that for any S value, magnetization S^z can be calculated using

$$S^z \quad \frac{(S \quad K)(1 \quad K)^{2S\ 1} \quad (1 \quad S \quad K)K^{2S\ 1}}{(1 \quad K)^{2S\ 1} \quad K^{2S\ 1}}. \tag{27}$$

b) Fermionic Green functions

Now let us use the fermionic Green functions. Taking $\quad = +1$ in (7), we have

$$C_{\mathbf{q}}^{(\ ,l)} \quad (S^z)^l S \ S \quad {}_{\mathbf{q}} \quad \frac{A_1^{(\ ,l)}}{e^{\ \mathbf{q}} \quad 1}, \tag{28}$$

Using the relation between anticommutator and commutator

$$A_1^{(\ ,l)}(\mathbf{q}) \quad A_1^{(\ ,l)} \quad 2C_{\mathbf{q}}^{(\ ,l)}\,, \tag{29}$$

one obtains

$$(S^z)^l S \ S \quad {}_{\mathbf{q}} \quad \frac{2\ (S^z)^l S \ S \quad {}_{\mathbf{q}}}{e^{\ \mathbf{q}} \quad 1} \quad \frac{A_1^{(\ ,l)}}{e^{\ \mathbf{q}} \quad 1} \tag{30}$$

which bring us back to (24). The conclusion is that for the asymmetric coupling, the fermionic Green function is exactly equivalent to the bosonic Green function.

2.2. Symmetric decoupling

In order to treat the reorientation of the magnetization, we need the following Green functions

$$G_{ij(\ )}^{(\ ,lm)}(\ ) \quad S_i\ ;(S_j^z)^l(S_j\ )^m \quad {}_{(\ )}\,, \tag{31}$$

where $\quad (\ ,\ ,z)$ takes care of all directions in space. The exact equation of motion are

$$G_{ij(\ )}^{(\ ,lm)}(\ ) \quad A_{ij(\ )}^{(\ ,lm)} \quad {}_{ij} \quad \sum_{k\ i} J_{ik}[\ S_i^z S_k\ ;(S_j^z)^l(S_j\ )^m \quad {}_{(\ )} \quad S_k^z S_i\ ;(S_j^z)^l(S_j\ )^m \quad {}_{(\ )}], \tag{32}$$

$$G_{ij(\ )}^{(z,lm)}(\ ) \quad A_{ij(\ )}^{(z,lm)} \quad {}_{ij} \quad \frac{1}{2}\sum_{k\ i} J_{ik} \quad (S_i\ S_k \quad S_k\ S_i\ );(S_j^z)^l(S_j\ )^m \quad {}_{(\ )} \tag{33}$$

with inhomogeneities

$$A_{ij(\ )}^{(\ ,lm)} \quad [S_i\ ,(S_j^z)^l(S_j\ )^m]\ . \tag{35}$$

The **symmetric decoupling** of the Green function is as follows

$$S_i\ S_k\ ;(S_j^z)^l(S_j\ )^m \quad _{(\ )} \quad S_i \quad S_k\ ;(S_j^z)^l(S_j\ )^m \quad _{(\ )} \quad S_k \quad S_i\ ;(S_j^z)^l(S_j\ )^m \quad _{(\ )}\ . \tag{36}$$

After the Fourier transform to momentum space, one obtains for a 3-dimensional Green function vector three equations of motion in the following matrix form

$$|\ \mathbf{I} \quad [\ (\mathbf{q})]|\ \mathbf{g}^{(lm)}(\mathbf{q},\ ) \quad \mathbf{A}^{(lm)}\ , \tag{37}$$

where

$$[\ (\mathbf{q})] \quad \begin{matrix} A & 0 & B \\ 0 & A & B \\ \frac{1}{2}B & \frac{1}{2}B & 0 \end{matrix}\ , \tag{38}$$

$$\mathbf{g}^{(lm)}(\mathbf{q},\ ) \quad \begin{matrix} g^{(\ ,lm)}(\mathbf{q},\ ) \\ g^{(\ ,lm)}(\mathbf{q},\ ) \\ g^{(z,lm)}(\mathbf{q},\ ) \end{matrix}\ , \tag{39}$$

$$\mathbf{A}^{(lm)} \quad \begin{matrix} A^{(\ ,lm)} \\ A^{(\ ,lm)} \\ A^{(z,lm)} \end{matrix} \tag{40}$$

with abbreviation

$/J,\ \mathbf{g}^{(lm)}(\mathbf{q},\ ) \quad J\mathbf{G}^{(lm)}(\mathbf{q},\ )\ , A \quad S^z\ [z \quad _{\mathbf{q}}],\ B \quad S^x\ [z \quad _{\mathbf{q}}]\ ,\ _{\mathbf{q}} \quad _j \quad e^{i\mathbf{q}.(\mathbf{a}_i\ \ \mathbf{a}_k)}$.

Matrix **I** is the unit matrix and z is the coordination number.

The eigenvalues $[\ (\mathbf{q})]$ of matrix are

$$_1 \quad 0,\quad _2(\mathbf{q}) \quad _{\mathbf{q}},\quad _3(\mathbf{q}) \quad _{\mathbf{q}},\ \text{where} \quad _{\mathbf{q}} \quad \sqrt{A^2 \quad B^2}\ , \tag{41}$$

It is seen that there is a zero eigenvalue. In this case equation (7) cannot be applied to the bosonic Green function directly. Now we employ the fermionic Green function, namely, taking $\ = 1$ in the equation (37). Between anticommutator and commutator inhomogeneities exists the following relation

$$\mathbf{A}_{\mathbf{q},\ \ 1}^{(lm)} \quad \mathbf{A}^{(lm)}_{\ \ 1} \quad 2\mathbf{C}_{\mathbf{q}}^{(lm)}\ , \tag{42}$$

Where $\mathbf{C}_{\mathbf{q}}^{(lm)}$ is the correlation vector

$$\mathbf{C}_{\mathbf{q}}^{(lm)} \quad \begin{matrix} (S^z)^l(S\ \ )^m S \quad _{\mathbf{q}} \\ (S^z)^l(S\ \ )^m S \quad _{\mathbf{q}} \\ (S^z)^l(S\ \ )^m S^z \quad _{\mathbf{q}} \end{matrix}\ . \tag{43}$$

It is important that the commutator inhomogeneities $\mathbf{A}^{(lm)}{}_{1}$ do not depend on the momentum **q**. We follow the eigenvalue method as mentioned in [4]. One starts with a transformation, which diagonalizes the matrix $[\ (\mathbf{q})]$ of equation (37)

$$\mathbf{U}|\ [\ (\mathbf{q})]|\mathbf{U}^{1}\qquad , \tag{44}$$

where is a diagonal matrix with eigenvalues $_{i}(i = 1,2,3)$, and the transformation matrix **U** and its inverse $\mathbf{U}^{-1}$ are obtained from the right eigenvectors of matrix $[\ (\mathbf{q})]$ as columns and from the left eigenvectors as rows, respectively. In our case the eigenvectors by which the transformation matrices **U** and $\mathbf{U}^{-1}$ are constructed can be given explicitly. They are

$$\mathbf{U}\quad \begin{matrix} \frac{B}{A} & \frac{_{\mathbf{q}}\ A}{B} & \frac{_{\mathbf{q}}\ A}{B} \\ \frac{B}{A} & \frac{_{\mathbf{q}}\ A}{B} & \frac{_{\mathbf{q}}\ A}{B} \\ 1 & 1 & 1 \end{matrix}\ ,\quad \mathbf{U}^{1}\quad \frac{1}{4\ {}^{2}_{\mathbf{q}}}\quad \begin{matrix} 2BA & 2BA & 4A^{2} \\ (\ _{\mathbf{q}}\ A)B & (\ _{\mathbf{q}}\ A)B & 2B^{2} \\ (\ _{\mathbf{q}}\ A)B & (\ _{\mathbf{q}}\ A)B & 2B^{2} \end{matrix}\ . \tag{45}$$

These matrices are normalized to unity: $\mathbf{U}\mathbf{U}^{-1} = \mathbf{U}^{-1}\mathbf{U} = \mathbf{1}$.

Multiplying the equation of motion (37) from the left $\mathbf{U}^{-1}$ and inserting $\mathbf{1} = \mathbf{U}\mathbf{U}^{-1}$ one finds

$$-\quad \mathbf{U}^{-1}\,\mathbf{g}^{(lm)}{}_{1}(\mathbf{q},\ )\quad \mathbf{U}^{-1}\,\mathbf{A}^{(lm)}{}_{1}$$

Defining $\ {}^{(lm)}_{\mathbf{q},\ \ 1}\quad \mathbf{U}^{1}\mathbf{g}^{(lm)}{}_{1}(\mathbf{q})$ and $\ {}^{(lm)}_{\mathbf{q},\ \ 1}\quad \mathbf{U}^{1}\mathbf{A}^{(lm)}_{\mathbf{q},\ \ 1}$ one obtains

$$-\quad {}^{(lm)}_{\mathbf{q},\ \ 1} = {}^{(lm)}_{\mathbf{q},\ \ 1}\,. \tag{47}$$

$^{(lm)}{}_{1}$ is a new vector of Green functions, each component *i* of which has but a single pole

$${}^{(lm,i)}_{\mathbf{q},\ \ 1}\quad \frac{{}^{(lm,i)}_{\mathbf{q},\ \ 1}}{\ \ _{i}}\,. \tag{48}$$

This is the important point and allows application of the spectral theorem to each component separately. This gives with $c^{(lm)}_{\mathbf{q}}\quad \mathbf{U}^{1}\mathbf{C}^{(lm)}_{\mathbf{q}}$

$$c^{(lm,i)}_{\mathbf{q}}\quad \frac{{}^{(lm,i)}_{\mathbf{q},}}{e^{\ \ _{i}}\ \ 1}\,. \tag{49}$$

We proceed with the anticommutator $\ = +1)$ and one obtains the original correlation vector $\mathbf{C}^{(lm)}_{\mathbf{q}}$ by multiplying from the left with **U**, i.e.

$$\mathbf{C}^{(lm)}_{\mathbf{q}} = \mathbf{R}_{\mathbf{q}}\,\mathbf{A}^{(lm)}_{\mathbf{q},\ \ 1}\,, \tag{50}$$

where $\mathbf{R}_{\mathbf{q}}\quad \mathbf{U}\mathbf{E}\mathbf{U}^{1}$ with matrix elements

$$R_{\mathbf{q},ij}\quad \sum_{k\ 1}^{3}\frac{U_{ik}U^{1}_{kj}}{e^{\ \ _{k}}\ \ 1}\,, \tag{51}$$

E is a diagonal matrix with matrix elements $E_{ij} \quad {}_{ij}(e^{\quad i} \quad 1)^{1}$. Using (42) one obtains the following set of equations

$$(\mathbf{I} \quad 2\mathbf{R}_{\mathbf{q}})\mathbf{C}_{\mathbf{q}}^{(lm)} = \mathbf{R}_{\mathbf{q}}\mathbf{A}^{(lm)}{}_{1}, \qquad (53)$$

or

$$\begin{pmatrix} \frac{A}{\quad_{\mathbf{q}}}\coth(\quad_{\mathbf{q}}/2) & 0 & \frac{B}{\quad_{\mathbf{q}}}\coth(\quad_{\mathbf{q}}/2) \\ 0 & \frac{A}{\quad_{\mathbf{q}}}\coth(\quad_{\mathbf{q}}/2) & \frac{B}{\quad_{\mathbf{q}}}\coth(\quad_{\mathbf{q}}/2) \\ \frac{B}{2\quad_{\mathbf{q}}}\coth(\quad_{\mathbf{q}}/2) & \frac{B}{2\quad_{\mathbf{q}}}\coth(\quad_{\mathbf{q}}/2) & 0 \end{pmatrix} \begin{pmatrix} C_{\mathbf{q}}^{(\quad,lm)} \\ C_{\mathbf{q}}^{(\quad,lm)} \\ C_{\mathbf{q}}^{(z,lm)} \end{pmatrix}$$

$$\begin{pmatrix} 1 \quad \frac{A}{\quad_{\mathbf{q}}}\coth(\quad_{\mathbf{q}}/2) & 0 & \frac{B}{\quad_{\mathbf{q}}}\coth(\quad_{\mathbf{q}}/2) \\ 0 & 1 \quad \frac{A}{\quad_{\mathbf{q}}}\coth(\quad_{\mathbf{q}}/2) & \frac{B}{\quad_{\mathbf{q}}}\coth(\quad_{\mathbf{q}}/2) \\ \frac{B}{2\quad_{\mathbf{q}}}\coth(\quad_{\mathbf{q}}/2) & \frac{B}{2\quad_{\mathbf{q}}}\coth(\quad_{\mathbf{q}}/2) & 0 \end{pmatrix} \begin{pmatrix} A_{1}^{(\quad,lm)} \\ A_{1}^{(\quad,lm)} \\ A_{1}^{(z,lm)} \end{pmatrix}, \qquad (54)$$

From (54) we have

$$C_{\mathbf{q}}^{(\quad,lm)}A \quad C_{\mathbf{q}}^{(z,lm)}B \quad A_{1}^{(\quad,lm)} \frac{1}{2} \quad_{\mathbf{q}}\coth(\quad_{\mathbf{q}}/2T) \quad \frac{1}{2}A \quad \frac{1}{2}BA_{1}^{(z,lm)}, \qquad (55)$$

$$C_{\mathbf{q}}^{(\quad,lm)}A \quad C_{\mathbf{q}}^{(z,lm)}B \quad A_{1}^{(\quad,lm)} \frac{1}{2} \quad_{\mathbf{q}}\coth(\quad_{\mathbf{q}}/2T) \quad \frac{1}{2}A \quad \frac{1}{2}BA_{1}^{(z,lm)}, \qquad (56)$$

$$BC_{\mathbf{q}}^{(\quad,lm)} \quad BC_{\mathbf{q}}^{(\quad,lm)} \quad \frac{1}{2}B(A_{1}^{(\quad,lm)} \quad A_{1}^{(\quad,lm)}) \quad _{\mathbf{q}}\coth(\quad_{\mathbf{q}}/2T)A_{1}^{(z,lm)}. \qquad (57)$$

Here we should emphasize the fact that matrices $\mathbf{C}_{\mathbf{q}}^{(lm)}$ and $\mathbf{R}_{\mathbf{q}}$ depend on **q**, but $\mathbf{A}^{(lm)}{}_{1}$ does not. The equations (56) include all the necessary information to calculate the statistical average of the spin operators.

Because the correlations are in real space, we have to perform a corresponding Fourier transformation $(S^{z})^{l}(S\quad)^{m}S \quad \frac{1}{N}\sum_{\mathbf{q}} (S^{z})^{l}(S\quad)^{m}S \quad_{\mathbf{q}}$. Fourier transform of equation (56) yields

$$C^{(\quad,lm)} \quad \frac{1}{N}\sum_{\mathbf{q}} \frac{B}{A}C_{\mathbf{q}}^{(z,lm)} \quad \frac{1}{2}A_{1}^{(\quad,lm)} \quad \frac{1}{2}A_{1}^{(\quad,lm)}\frac{1}{N}\sum_{\mathbf{q}} \frac{\quad_{\mathbf{q}}}{A}\coth\frac{\quad_{\mathbf{q}}}{2T} \quad \frac{1}{2}A_{1}^{(z,lm)}\frac{1}{N}\sum_{q}\frac{B}{A}. \qquad (58)$$

Putting this into the Fourier transform of (55) one can eliminate the term $\frac{1}{N}\sum_{\mathbf{q}}\frac{B}{A}C_{\mathbf{q}}^{(z,lm)}$. One obtains

$$C^{(\quad,lm)} \quad C^{(\quad,lm)} \quad \frac{1}{2}(A_{1}^{(\quad,lm)} \quad A_{1}^{(\quad,lm)}) \quad \frac{1}{2}(A_{1}^{(\quad,lm)} \quad A_{1}^{(\quad,lm)})\frac{1}{N}\sum_{\mathbf{q}}\frac{\quad_{\mathbf{q}}}{A}\coth\frac{\quad_{\mathbf{q}}}{2T}. \qquad (59)$$

The Fourier transform of equation (57) can be done directly and gives

$$C^{(\ ,lm)} \quad C^{(\ ,lm)} \quad \frac{1}{2}(A_1^{(\ ,lm)} \quad A_1^{(\ ,lm)}) \quad A_1^{(z,lm)} \frac{1}{N} \sum_{\mathbf{q}} \frac{\mathbf{q}}{B} \coth \frac{\mathbf{q}}{2T} \ . \tag{60}$$

To elucidate the equations (59) and (60) we derive the explicit expressions for $S = 1/2$. We need determine the correlations $C^{(\ ,lm)}$ and the inhomogeneities $A_1^{(\ ,lm)}$ ($= +,-, z$) for $l = 0$ and $m = 1$:

$$C^{(\ ,01)} \quad (S^z)^0(S\ )^1 S \qquad S\ S \quad 1/2 \quad S^z\ ,\ C^{(\ ,01)} \quad (S^z)^0(S\ )^1 S \qquad S\ S \quad 0\ ,$$

$$A_1^{(\ ,01)} \quad [S\ ,S\ ]\ _1 \quad 2\ S^z\ ,\ A_1^{(\ ,01)} \quad [S\ ,S\ ]\ _1 \quad 0\ ,$$

$$A_1^{(z,01)} \quad [S^z, S\ ]\ _1 \quad S \qquad S^x\ .$$

Inserting these into (59) and (60) one finds

$$S^z \quad \frac{1}{2\ \ _1(T\ )}\ , \qquad S^x \quad \frac{1}{2\ \ _2(T\ )}\ , \tag{61}$$

where

$$_{1(2)}(T\ ) \quad \frac{1}{N} \sum_{\mathbf{q}} \frac{\mathbf{q}}{A(B)} \coth \frac{\mathbf{q}}{2T} \ . \tag{62}$$

These are two equations which determine the two unknowns: S^x and S^z .

For $S = 1$ one needs equations for ($l = 0$, $m = 1$), ($l = 1$, $m = 1$), ($l = 0$, $m = 2$), ($l = 0$, $m = 3$). This yields 8 equations for the eight unknowns. Solving these equations we obtain for S^z and S^x the following expressions

$$S^z \quad \frac{4\ \ _1(T\ )\ \ _2^2(T\ )}{\ _1^2(T\ )\quad \ _2^2(T\ )\ \ 3\ \ _1^2(T\ )\ \ _2^2(T\ )}, \tag{63}$$

$$S^x \quad \frac{4\ \ _2(T\ )\ \ _1^2(T\ )}{\ _1^2(T\ )\quad \ _2^2(T\ )\ \ 3\ \ _1^2(T\ )\ \ _2^2(T\ )}. \tag{64}$$

For $S = 3/2$ one needs equations for ($l = 0$, $m = 1$), ($l = 1$, $m = 1$), ($l = 0$, $m = 2$), ($l = 0$, $m = 3$), ($l = 1$, $m = 2$), ($l = 1$, $m = 3$), a ($l = 2$, $m = 2$). This yields 14 equations for the eight unknowns. Solving these equations we obtain for and the following expressions

$$S^z \quad \frac{5(58\ \ _1^2\quad 58\ \ _2^2\quad 115\ \ _1\ \ _2^2\quad 150\ \ _1^2\ \ _2^2)}{2(92\ \ _1^2\quad 178\ \ _1^3\quad 92\ \ _2^2\quad 178\ \ _1\ \ _2^2\quad 115\ \ _1^2\ \ _2^2\quad 150\ \ _1^3\ \ _2^2)}, \tag{65}$$

$$S^x \quad \frac{5(58\ \ _1^3\quad 58\ \ _1\ \ _2^2\quad 115\ \ _1^2\ \ _2^2\quad 150\ \ _1^3\ \ _2^2)}{2(92\ \ _1^2\ \ _2\quad 178\ \ _1^3\ \ _2\quad 92\ \ _2^3\quad 178\ \ _1\ \ _2^3\quad 115\ \ _1^2\ \ _2^3\quad 150\ \ _1^3\ \ _2^3)}. \tag{66}$$

From (61), (63), (64) and (65), (66) the values of the total magnetization $M(T\ )$ and the equilibrium polar angle of the magnetization are determined for $S = 1/2$, $S = 1$, and $S = 3/2$, respectively:

$$M^2(T\ ) \quad S^{x\ 2} \quad S^{z\ 2}\ , \tag{67}$$

$$\arctan \frac{S^x}{S^z} . \tag{68}$$

3. Conclusion

The presented fermionic Green function method has recently been successfully applied to treat magnetic reorientation in ferromagnetic thin films [4], [7] and in ferromagnetic monolayers [8], [9]. In reference [10] within fermionic Green functions method the properties of he transversal Heisenberg model is considered. The many-body Green function theory allows calculations the magnetic properties of a Heisenberg ferromagnet (antiferromagnet) over the entire temperature range of interest in contrast to other methods, which are only valid at low (Holstein-Primakoff approach) or high temperatures (high temperature expansions). We have used the symmetric and antisymmetric Tyablikov (RPA) decoupling for the exchange interaction term.

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References

[1] D. Li, M. Freitag, J. Pearson, Z. Q. Qiu, S.D. Bader: J. Appl. Phys. **76** (1994) 6425.
[2] M. Farle, W. Platow, A. N. Anisimov, P. Poulopoulos, K. Baberschke: Phys. Rev. B **56** (1997) 510.
[3] V. Ramakrishnan, T. Tanaka: Phys. Rev. B **16** (1977) 422.
[4] P. Fröbrich, P. J. Jensen, P. J. Kuntz, A. Ecker: Eur. Phys. J. B **18** (2000) 579.
[5] H. Wang, K. Chen: Int. J. Mod. Phys. B **16** (2002) 3803.
[6] H. B. Callen: Phys. Rev. **130** (1963) 890.
[7] P. Fröbrich, P. J. Kuntz: Eur. Phys. J. B **32** (2000) 445.
[8] V. Ilkovič: Phys. Stat. Sol. (b) **241** (2004) 420.
[9] V. Ilkovič, J. Kecer: Czech. J. Phys. **54** (2004) (to be published).
[10] V. Ilkovič, J. Kecer: Acta Physica Slovaca **54** (2004) 465.