Magnetic Properties of Dilute Alloys: Equations for Magnetization and its Structural Fluctuations

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Abstract

The dilute Heisenberg ferromagnet is studied taking into account fluctuations of magnetization caused by disorder. A self–consistent system of equations for magnetization and its mean quadratic fluctuations is derived within the configurationally averaged two–time temperature Green’s function method. This system of equations is analysed at low concentration of non–magnetic impurities. Mean relative quadratic fluctuations of magnetization are revealed to be proportional to the square of concentration of impurities.
Introduction

The method of configurationally averaged Green’s function developed by Kaneyoshi \[1\] to study a dilute ferromagnet was used successfully by several authors \[2\] to describe disordered magnetic systems. One of the most frequently used approximations within the frames of this method is neglecting the fluctuations of magnetization caused by disorder \[3, 4\]. Note that at zero temperature the magnetization for Heisenberg model tends to saturation and fluctuations are suppressed.

In paper \[1\] it was shown that taking into account the structural fluctuations of magnetization is necessary in order to explain the anomalous behaviour of spin–wave stiffness constant in amorphous ferromagnets. It was assumed that the structural fluctuations of magnetization at each site are statistically independent and are governed by a Gauss distribution function. In order to obtain quantitative results one needs to take into account the connection of the structural fluctuations of magnetization at each site with the fluctuations of structure. In our previous work \[6\] this relation was obtained within the framework of mean–field approximation. It allowed one to analyse quantitatively the spin–wave spectrum of amorphous ferromagnets.

In the present paper we estimate the dependence of structural fluctuations of magnetization on the concentration of non–magnetic sites in a dilute ferromagnet. We suggest a self–consistent set of equations for magnetization and its spectrum of amorphous ferromagnets.

1 Configurationally Averaged Green’s Functions

Let us consider a structurally disordered system of \(N\) atoms in the volume \(V\) which is described by the isotropic Heisenberg Hamiltonian

\[
H = -\frac{1}{2} \sum_{i,j} J_{ij} n_i n_j S_i S_j - \hbar \sum_j n_j S_j^z,
\]

where \(J_{ij} = J(|\mathbf{R}_i - \mathbf{R}_j|)\) is the exchange integral describing the interaction between the \(i\)th and \(j\)th atoms, \(S_i\) is the spin operator of the \(i\)th atom, \(\hbar\) is the external magnetic field, \(n_i\) is a random variable taking the value of 1 or 0 according to whether or not the site \(i\) is occupied by a magnetic atom.

The Fourier–component of retarding two–time temperature Green’s function

\[
\ll l\ll l' \gg_t \equiv \ll n_i S_i^+ | n_{l'} S_{l'}^- \gg_t \equiv -i\delta(t) \ll [S_i^+(t), S_{l'}^-(0)] \gg n_l n_{l'}
\]

satisfies within the Tyablikov approximation the equation of motion

\[
(E - \hbar) \ll l\ll l' \gg_E = 2\delta_{l,l'} x_l + \sum_{j \neq l} J_{ij} (x_j \ll l\ll l' \gg_E - x_l \ll j l' \gg_E),
\]

where \(x_i = \ll S_i^z \gg n_i\) is the magnetization of the \(i\)th site and \(x = \ll x \gg t\) is the mean magnetization. The overbar means the averaging over configurations but due to self–averaging of magnetization we can write

\[
x = \frac{1}{N} \sum_i x_i = \frac{1}{N} \sum_i \ll S_i^z \gg n_i = N_m \frac{1}{N_m} \sum_{i(n_i=1)} \ll S_i^z \gg = n\ll S_i^z \gg \equiv n\sigma,
\]

where double overline means the averaging over the magnetic sites only. Extracting fluctuations \(\xi_i = x_i - x\) and coming to a momentum space

\[
\ll q|q' \gg = \frac{1}{N} \sum_{i,j=1}^N e^{-i(q\mathbf{R}_i - q'\mathbf{R}_j)} \ll i|j \gg, \quad \xi_q = \frac{1}{\sqrt{N}} \sum_{j=1}^N \xi_j e^{-i q\mathbf{R}_j},
\]

we get

\[
(E - E_0(q)) \ll q|q' \gg = 2\varepsilon_0 (q - q') + \frac{2}{\sqrt{N}} \xi_{q-q'} + \frac{1}{\sqrt{N}} \sum_k A(q,k) \xi_{q-k} \ll k|q' \gg,
\]

\[
(1.4)
\]
where \( J(q) = \sum R e^{-i q R} \) is a Fourier transform of exchange integral, \( E_0(q) = h + x A(q, q) \) is the spin–wave spectrum of a non–dilute crystal and the notation \( A(q, k) = J(q - k) - J(k) \) is introduced for convenience. All sums in equation (1.4) and hereafter in the reciprocal space are taken over the Brillouin zone. It is worth while remembering that there is just a lattice and therefore all Fourier transformations from the real space to momentum space are reversible.

Note that \( x_i \) or \( \xi_i \) include fluctuations of structure \( n_i \) as well as fluctuations of magnetization \( < S_i^z > \). It is convenient to rewrite equation (1.4) in the matrix form:

\[
G = G^0 + G^0 \rho + G^0 Q G,
\]

(1.5)

where

\[
G_{q, q'} = \langle q | q' \rangle \]

is the unaveraged Green’s function,

\[
G^0_{q, q'} = \frac{2 \pi \delta_{q, q'}}{E - E_0(q)}
\]

is the zero–approximation Green’s function,

\[
\rho_{q, q'} = \frac{\xi_q \xi_{q'}}{\sqrt{N x}}
\]

is the matrix of relative fluctuations of magnetization and the matrix

\[
Q_{q, q'} = \frac{A(q, q')}{2} \rho_{q, q'}
\]

is proportional to relative fluctuations of magnetization and depends on the exchange interaction between spins. The zero–approximation Green’s function of the dilute system has the same form as in the non–dilute case with the only difference that the mean magnetization \( x = n \sigma \) must be substituted in place of \( \sigma \).

Averaging equation (1.5) over configurations we obtain

\[
\overline{G} = G^0 + G^0 \overline{G} G.
\]

(1.6)

To obtain an equation for the new unknown Green’s function \( \overline{G} G \) we need to multiply equation (1.5) by the matrix \( G^0 Q \) and to average the product over configurations. Substituting the result in expression (1.4) we get another expression for \( \overline{G} \):

\[
\overline{G} = G^0 + G^0 \overline{G} G^0 \rho + G^0 \overline{G} G^0 Q \overline{G} G,
\]

(1.7)

which contains the matrix \( \overline{G} G^0 Q \overline{G} G \). We can obtain the equation for this averaged product in the same way and continuing this iteration procedure we can get similarly as it is described in [2] the expression for the configurationally averaged Green’s function

\[
\overline{G} = \left( 1 - G^0 \sum_{i=1}^{\infty} \Delta Q, i \right)^{-1} G^0 \left( 1 + \sum_{i=1}^{\infty} \Delta Q, i \rho \right),
\]

(1.8)

where

\[
\Delta Q, i = Q, i - \overline{Q}, \quad Q, 0 = QG^0, \quad Q, i = \Delta Q, i-1 QG^0 \text{ for } i > 1.
\]

All three factors in equation (1.8) are diagonal matrices in the momentum space and we can rewrite this expression as

\[
[\overline{G}]_q = \frac{[G^0]_q \left( 1 + \sum_{i=1}^{\infty} \Delta Q, i \rho \right)}{1 - [G^0]_q \sum_{i=1}^{\infty} \Delta Q, i \rho},
\]

(1.9)

where \([ \ldots ]_q \equiv [ \ldots ]_q q\) is a diagonal element of the matrix.

Let us consider other Green’s function \( G_1 = G \rho \) which we will use further. To obtain the equation for this function let us multiply the equation (1.3) by \( \rho \). We get

\[
G_1 = G^0 (\rho + \rho^2) + G^0 Q G_1.
\]

(1.10)

An averaged value of \( G_1 \) obtained within the similar iteration procedure has the following form

\[
\overline{G}_1 = \left( 1 - G^0 \sum_{i=1}^{\infty} \Delta Q, i \right)^{-1} G^0 \left( \rho^2 + \sum_{i=1}^{\infty} \Delta Q, i (\rho + \rho^2) \right).
\]

(1.11)
\[ [G_1]_q = \frac{[G^0]_q \left( [p^2]_q + \sum_{i=1}^\infty [\Delta Q_i (\rho + p^2)]_q \right)}{1 - [G^0]_q \sum_{i=1}^\infty [\Delta Q_i Q_i]_q} \]  

(1.12)

for the diagonal elements in the momentum space.

Note that the matrix \( \rho^2 \) is proportional to the unit matrix:

\[ \rho^2_q = \frac{1}{N} \sum_k \xi_{k-k-q} x^2 - \frac{1}{N} \sum_l \xi^2_l x^2 = \xi^2 x^2. \]  

(1.13)

### 2 Equations for Magnetization and its Structural Quadratic Fluctuation

As was shown by Kaneyoshi in [4] the averaged Green’s function \( \overline{G} \) can be expressed approximately in terms of mean magnetization \( x \) and its mean quadratic fluctuations \( \xi^2 \). To obtain equations describing these quantities let us consider the equation for a mean moment at the \( l \)th site that expresses it in terms of non–averaged Green’s function in the energy representation \( \ll l | l \gg E \). In a standard way we obtain

\[ x_l = \frac{1}{2} n_l - \int_{-\infty}^{\infty} \frac{dE}{e^{3E} - 1} \left( -\frac{1}{\pi} \Im \ll l | l \gg E + i0 \right). \]  

(2.1)

Averaging this equation over configuration we obtain the equation for mean magnetization

\[ x = \frac{1}{2} n - \int_{-\infty}^{\infty} \frac{dE}{e^{3E} - 1} \left( -\frac{1}{\pi N} \Im \text{Sp} \overline{G}(E + i0) \right), \]  

(2.2)

where we took into account that the averaged one–site Green’s function does not depend on the number of the site:

\[ \ll l | l \gg = \frac{1}{N} \sum_q \ll q | q \gg = \frac{1}{N} \text{Sp} \overline{G}. \]

Subtracting the averaged equation (2.2) from the non–averaged one (2.1), multiplying the result by the fluctuation \( \xi_l \) and averaging the product over configurations we obtain the following equation for quadratic fluctuations

\[ \overline{\xi^2} = \frac{1}{2} \Delta n \xi - \int_{-\infty}^{\infty} \frac{dE}{e^{3E} - 1} \left( -\frac{1}{\pi N} \Im \text{Sp} \overline{G}_1(E + i0) \right). \]  

(2.3)

It is easy to prove that

\[ \Delta n \xi = (n_l - n)(n_l < S^z_l > - x) = (1 - n) x \]

and

\[ \overline{\xi_l | l | l} = \frac{x}{N} \text{Sp} \overline{G}_1. \]

Substituting these two equations in (2.3) we obtain finally

\[ \overline{\xi^2} = x \left( \frac{1}{2} (1 - n) - \int_{-\infty}^{\infty} \frac{dE}{e^{3E} - 1} \left( -\frac{1}{\pi N} \Im \text{Sp} \overline{G}_1(E + i0) \right) \right). \]  

(2.4)

Let us consider the meaning of mean quadratic fluctuations \( \overline{\xi^2} \) more closely. We find that

\[ \overline{\xi^2} = (n_l < S^z_l >)^2 - x^2 = n < S^z_l >^2 - x^2 = n < S^z >^2 - \sigma^2 + \frac{1 - n}{n} x^2 = n(\Delta \sigma)^2 + \frac{1 - n}{n} x^2, \]  

(2.5)
where the first term in the final expression corresponds just to the fluctuations of mean moment of magnetic atoms while the second term corresponds to the fluctuations of structure. Therefore it is convenient to divide these two terms. We can easily find that the mean quadratic fluctuations of moments of magnetic atoms have the form

\[
\langle \Delta \sigma^2 \rangle = \sigma \left( \frac{1}{2} (1 - n) - \frac{1 - n}{n} x - \int_{-\infty}^{\infty} \frac{dE}{e^{\beta E} - 1} \left( -\frac{1}{\pi N} \text{Sp} G_1(E + i0) \right) \right). \tag{2.6}
\]

We can use the equation for mean magnetization \(2.2\) to rewrite this equation in the following form

\[
\langle \Delta \sigma^2 \rangle = \sigma \int_{-\infty}^{\infty} \frac{dE}{e^{\beta E} - 1} \left( -\frac{1}{\pi N} \text{Sp} G_2(E + i0) \right), \tag{2.7}
\]

where we have introduced the new Green’s function

\[
G_2 = \frac{1 - n}{n} G - G_1 \tag{2.8}
\]

The averaged value of this Green’s function can be derived from equations \(1.8\) and \(1.11\) as follows

\[
G_2 = \left( 1 - G_0 \sum_{i=1}^{\infty} \Delta Q_i Q \right) \left( -\frac{\langle \Delta \sigma^2 \rangle}{n \sigma^2} + \frac{1 - n}{n} \sum_{i=1}^{\infty} \Delta Q_i \rho \right) - \sum_{i=1}^{\infty} \Delta Q_i (\rho + \rho^2), \tag{2.9}
\]

or

\[
\left[ \frac{\langle \sigma^2 \rangle}{q} \right] = \frac{\cancel{[G_0]^0} \left( -\frac{\langle \Delta \sigma^2 \rangle}{n \sigma^2} + \frac{1 - n}{n} \sum_{i=1}^{\infty} \Delta Q_i \rho \right) q - \sum_{i=1}^{\infty} \Delta Q_i (\rho + \rho^2) q}{1 - \cancel{[G_0]^0} \sum_{i=1}^{\infty} \Delta Q_i Q q}, \tag{2.10}
\]

for the diagonal elements in the momentum space. Here we have used the fact that

\[
\frac{\rho^2}{x^2} = \frac{\langle \Delta \sigma^2 \rangle}{n \sigma^2} + \frac{1 - n}{n}. \tag{2.11}
\]

It is convenient to come to the dimensionless variables

\[
\mathcal{E} = \frac{E - h}{x J(0)}, \quad \hat{\beta} = \beta J(0), \quad \hat{h} = \frac{h}{J(0)}, \quad \tilde{G}_\alpha = J(0) G_\alpha. \tag{2.12}
\]

Then the equations for the magnetization \(x\) and the mean quadratic fluctuations of magnetization of magnetic subsystem \(\langle \Delta \sigma^2 \rangle\) take the form

\[
x = n \left( \frac{1}{2} + 2 \int_{-\infty}^{\infty} \frac{d\mathcal{E}}{e^{\hat{\beta}(\mathcal{E} x + \hat{h})} - 1} g(\mathcal{E}) \right)^{-1}, \tag{2.13}
\]

\[
\frac{\langle \Delta \sigma^2 \rangle}{n \sigma^2} = 2 \int_{-\infty}^{\infty} \frac{d\mathcal{E}}{e^{\hat{\beta}(\mathcal{E} x + \hat{h})} - 1} g_2(\mathcal{E}) \tag{2.14}
\]

where

\[
g_\alpha(\mathcal{E}) = -\frac{1}{2\pi N} \text{Sp} \tilde{G}_\alpha (\mathcal{E} + i0). \tag{2.15}
\]

We can assume that the spectral density \(g(\mathcal{E})\) does not depend on the mean magnetization \(x\), similarly as in the case of the non–dilute system. Then substituting zero external field into equation \(2.12\) for magnetization \(x\) and looking for the limit of the zero magnetization we obtain in a standard way the following equation for critical temperature

\[
\frac{T_c}{J(0)} = n \int_{-\infty}^{\infty} \frac{d\mathcal{E}}{\mathcal{E}} g(\mathcal{E}). \tag{2.16}
\]

\[\text{4}\]
To solve this set of equations self-consistently we need to express the averaged Green’s functions \( \overline{G} \) and \( \overline{G_2} \) in terms of the magnetization \( x \) and quadratic fluctuations of the magnetic subsystem \( \overline{\Delta \sigma^2} \) only. In the following section we consider the limit of low concentration of nonmagnetic impurities satisfying this condition. The analysis of different approximations allowing to reach this aim for any concentration of nonmagnetic impurities will be the subject of further works.

3 Low Concentration of Nonmagnetic Impurities

Let us estimate the value

\[
\rho_{q,k_1,k_2,\ldots,k_m} = \frac{1}{N^m} \sum_{l_1,\ldots,l_m} \exp \left( -i \sum_{j=1}^m \iota_j (k_j - k_{j-1}) \right) \overline{\xi_{l_1} \cdots \xi_{l_m}} \bigg|_{k_0=k_m=q} \tag{3.1}
\]

we need to calculate to obtain the averaged Green’s functions. For the low concentration of non-magnetic atoms we can neglect the correlations of fluctuations on different sites supposing

\[
\overline{\xi_{l_1}^{m_1} \cdots \xi_{l_j}^{m_j}} = \overline{\xi_{l_1}^{m_1}} \cdots \overline{\xi_{l_j}^{m_j}}. \tag{3.2}
\]

The only values we need to calculate within this approximation are \( \overline{\xi_q^m} \). It is easy to show that

\[
\overline{\xi^m} = (1 - n)(-x)^m + n(\Delta \sigma + (1 - n)\sigma)^m = (1 - n)(-x)^m + n(\Delta \sigma)^m + o(1 - n). \tag{3.3}
\]

Let us remind that for the Gauss distribution of the random value \( \zeta \)

\[
(\Delta \zeta)^{2m} = (2m - 1)!!(\Delta \zeta)^2, \quad (\Delta \zeta)^{2m+1} = 0. \tag{3.4}
\]

We don’t know the distribution law for magnetization fluctuations but we can suppose that the other than quadratic fluctuations are small enough to be neglected within the linear as to the concentration of non-magnetic atoms approximation

\[
\overline{(\Delta \sigma)^m} = o \left( \overline{(\Delta \sigma)^2} \right), \quad m > 2. \tag{3.5}
\]

Hereafter we shall neglect higher than quadratic moments of magnetization of the magnetic subsystem. Within the made approximation we obtain

\[
\rho_{q,k_1,k_2,\ldots,k_m} \approx \frac{1}{N^{m-1}} (\overline{\xi_q})^m + \tag{3.6}
\]

\[
\frac{1}{N^{m-2}} \sum_{j=2}^{m-2} \left( \overline{\xi_q} \right)^j \left( \overline{\xi_q} \right)^{m-j} \sum_{\{\lambda\}_{m-1}} \delta_{\lambda} \left( q - k_{m-1} + \sum_{j=1}^{m-1} (k_{j+1} - k_j) \right) \bigg|_{k_0=q},
\]

where \( \{\lambda\}_{m} = \{\lambda_1, \ldots, \lambda_j\} \subset \{1, \ldots, m\} \) and \( \delta_{\lambda} \equiv \delta_{\lambda,0} \) is Kronecker’s symbol. The first term in the right hand side of expression (3.6) corresponds to the one-site approximation and the second one corresponds to the two-site approximation where we have neglected possible correlations of the fluctuations on different sites.

Let us calculate the Green’s functions \( \overline{G} \) and \( \overline{G_2} \) taking into account only the terms linear as to the concentration of nonmagnetic atoms. Within the made approximations the series in expressions (1.9) and (2.10) for the averaged Green’s functions \( \overline{[G]}_q \) and \( \overline{[G_2]}_q \) can be summed up. Indeed

\[
\sum_{i=1}^{\infty} [\Delta \mathcal{Q}_i \rho]_q = \sum_{i=1}^{\infty} ([\mathcal{Q}^{(n)}_i \rho]_q + o(1 - n) \approx \tag{3.7}
\]

\[
\sum_{i=1}^{\infty} N^i \sum_{k_1,\ldots,k_i} B_{q,k_1,k_2,\ldots,k_{i-1},k_i} \rho_{q,k_1,k_2,\ldots,k_{i-1},k_i} \approx \sum_{i=1}^{\infty} \sum_{k} \left( \overline{\xi_q} \right)^{i+1} [B^{(i)}_1]_q, k.
\]
Thus we obtain the approximate expressions for the averaged Green’s functions

\[ \sum_{i=1}^{\infty} \langle \Delta Q_i \rho \rangle_q \approx \sum_{k=1}^{\infty} \left( (1-n)(-1)^{i+1} + n \frac{\langle \Delta \sigma \rangle^{i+1}}{\sigma^2} \right) [B']_{q,k} \approx \frac{(1-n) \sum_{k} [B(1+B)^{-1}]_{q,k} + \langle \Delta \sigma \rangle^2 \sum_{k} B_{q,k}}{(3.8)} \]

In a similar way we can estimate other series as follows

\[ \sum_{i=1}^{\infty} \langle \Delta Q_i \rho^2 \rangle_q \approx -(1-n) \sum_{k} [B(1+B)^{-1}]_{q,k} \]  

(3.10)

Thus we obtain the approximate expressions for the averaged Green’s functions \( \overline{G} \) and \( \overline{G}_2 \) in terms of the mean magnetization \( x \) and structural magnetic fluctuations of magnetic subsystem \( \frac{\langle \Delta \sigma \rangle^2}{\sigma^2} \) only.

\[ \overline{[G]}_q = 2 \frac{1 + \langle \Delta \sigma \rangle^2 \sum_{k} B_{q,k} + (1-n) \sum_{k} [B(1+B)^{-1}]_{q,k}}{\mathcal{E} - \mathcal{E}_0(q) - \frac{\langle \Delta \sigma \rangle^2}{\sigma^2} [BA]_{q,q} - (1-n) [B(1+B)^{-1}A]_{q,q}} \]  

(3.11)

and

\[ \overline{[G]}_2 = 2 \frac{\overline{[G]}_q - \langle \Delta \sigma \rangle^2 (1 + \sum_{k} B_{q,k})}{\mathcal{E} - \mathcal{E}_0(q) - \frac{\langle \Delta \sigma \rangle^2}{\sigma^2} [BA]_{q,q} - (1-n) [B(1+B)^{-1}A]_{q,q}} . \]  

(3.12)

Substituting expression \( \overline{[G]}_2 \) in equation (2.14) we can find that it gives us zero solution for the fluctuations \( \frac{\langle \Delta \sigma \rangle^2}{\sigma^2} \).

It means that this value is of a higher order as to concentration of non–magnetic impurities and it should be neglected within the linear approximation. Thus we can rewrite the Green’s function \( \overline{G} \) in the form

\[ \overline{[G]}_q = 2 \frac{1 + (1-n)C(\mathcal{E}, q)}{\mathcal{E} - \mathcal{E}_0(q) - (1-n)\Sigma(\mathcal{E}, q) \mathcal{E}_0(q)} , \]

(3.13)

where

\[ C(\mathcal{E}, q) = \sum_{k} [B(1+B)^{-1}]_{q,k} \]  

(3.14)

\[ \Sigma(\mathcal{E}, q) = [B(1+B)^{-1}A]_{q,q} . \]

(3.15)

This expression contains neither magnetization nor its fluctuations. The problem of calculating the inverse matrix \( (1+B)^{-1} \) is well known in theory of crystals with impurities and similar matrices were calculated in \( \overline{G} \) and \( \overline{G}_2 \). We present a simple way of calculating the functions \( C \) and \( \Sigma \) for the d–dimensional simple cubic lattice with the nearest neighbours interaction in appendix A.

From the poles of the averaged function \( \overline{G} \) we can obtain the equation for the spectrum of spin excitations

\[ \mathcal{E} - \mathcal{E}_0(q) - (1-n)\Sigma(\mathcal{E}, q) = 0 \]  

(3.16)
We present here only the long-wave solution of this equation for the simple cubic lattice with the nearest neighbours interaction

\[ E \approx Dq^2 = xJa^2 \left( 1 - 2(1 - n) \frac{I_{x^2}(d)}{1 - I_{x^2}(d)} \right) q^2 = \sigma Ja^2 n \left( 1 - 2(1 - n) \frac{I_{x^2}(d)}{1 - I_{x^2}(d)} \right) q^2 = \sigma Ja^2 \left( 1 - (1 - n) \frac{1 + I_{x^2}(d)}{1 - I_{x^2}(d)} + o((1 - n)^2) \right) q^2, \]

where \( J \) is the exchange integral for the nearest sites, \( a \) is the lattice constant, \( d \) is the dimensionality of lattice. The integral

\[ I_{x^2}(d) = \frac{1}{(2\pi)^d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \sin^2(x_1) \sum_{\mu=1}^{d} (1 - \cos(x_\mu)) \]

is smaller than the one for all the dimensions except \( d = 1 \). In the one-dimensional case the denominator of the second term in the expression for spectrum \((3.17)\) diverges that corresponds to the fact that spin-waves cannot propagate in the one-dimensional ferromagnet with the nearest neighbours interaction at any dilution. For the dimensions \( d \geq 2 \) the spin-wave stiffness constant \( D \) in expression \((3.17)\) tends to zero while the concentration of the magnetic sites \( n \) decreases to the percolation limit \( n_c \) which within the linear as to the concentration of nonmagnetic impurities approximation takes the form

\[ n_c = 1 - \frac{1 - I_{x^2}(d)}{1 + I_{x^2}(d)} = \frac{2I_{x^2}(d)}{1 + I_{x^2}(d)} \quad (3.19) \]

Note that we can reduce integral \((3.18)\) to the one-dimensional form

\[ I_{x^2}(d) = \int_{0}^{\infty} e^{-dt} \frac{I_1(t)}{t} \frac{I^d-1(t)}{t} dt, \quad (3.20) \]

where we have used the transformation

\[ \frac{1}{\sum_{\mu=1}^{d} (1 - \cos(x_\mu))} = \int_{0}^{\infty} \exp \left( -t \sum_{\mu=1}^{d} (1 - \cos(x_\mu)) \right) dt \quad (3.21) \]

and the following properties of the modified Bessel functions \( I_v(t) \)

\[ \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{it\cos(x)} \cos(nx) dx = I_n(t), \quad \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{it\cos(x)} \sin^2 x dx = \frac{I_0(t) - I_2(t)}{2} = \frac{I_1(t)}{t}. \quad (3.22) \]

As the expression for the percolation threshold \((3.19)\) is obtained within the linear over \( 1 - n \) approximation it shall give reliable results for low dimensions when \( 1 - n_c \) is small but we can not expect any reliability for large \( d \) when \( (1 - n_c) \rightarrow 0 \). Indeed, for \( d \rightarrow \infty \) the percolation threshold \( n_c \rightarrow \frac{1}{2} \) that does not coincide with the Bethe expression \( n_c^B = \frac{1}{2d-1} \) which is an asymptotic of the percolation threshold at large \( d \). Nevertheless as we can see from the Table I the results for the percolation threshold obtained from \((3.19)\) are better for \( d = 2 \) and \( d = 3 \) than the ones obtained within the Bethe-lattice approach. One can find some results of the latter approach for the theory of dilute ferromagnets in [10, 11, 12].

Table I. Percolation thresholds of the sc lattice from this work \( n_c \), in comparison with the "exact estimates" \( n_c^e \) taken from [13] and Bethe expression \( n_c^B = 1/(q - 1) \). For the sc lattice the number of the nearest neighbours \( q = 2d \).
| Dimension | $n_c^c$ | $n_c^B$ | $n_c$ |
|-----------|---------|---------|-------|
| $d = 1$   | 1       | 1       | 1     |
| $d = 2$   | 0.5928  | 0.3 (   | 0.53306 |
| $d = 3$   | 0.3116  | 0.2     | 0.34689 |
| $d = 4$   | 0.197   | 0.14 (   | 0.25585 |
| $d = 5$   | 0.141   | 0.1     | 0.20286 |
| $d = 6$   | 0.107   | 0.09     | 0.16824 |
| $d = 7$   | 0.089   | 0.076923 | 0.14380 |
| $d = 8$   | 0.0 (6) | 0.12561 |
| $d = 9$   | 0.058823 | 0.11153 |
| $d = 10$  | 0.052632 | 0.10030 |
| $d = 100$ | 0.0050251 | 0.01000 |

Let us write an explicit expression for the spectral density $g(\mathcal{E})$ which we need to calculate magnetization (2.13) and critical temperature (2.16)

\[
g(\mathcal{E}) = \frac{1}{N} \sum_{\mathbf{q}} g(\mathcal{E}, \mathbf{q}),
\]

\[
g(\mathcal{E}, \mathbf{q}) \equiv -\frac{1}{2\pi} \text{Im}[G]_\mathbf{q}(\mathcal{E} + i0) = \frac{1}{\pi} \frac{(1 - n)\Sigma''(\mathcal{E}, \mathbf{q}) + F(\mathcal{E}, \mathbf{q})}{(\mathcal{E} - \mathcal{E}_0(\mathbf{q}) - (1 - n)\Sigma'(\mathcal{E}, \mathbf{q}))^2 + ((1 - n)\Sigma''(\mathcal{E}, \mathbf{q}))^2},
\]

where

\[
F(\mathcal{E}, \mathbf{q}) = (1 - n)C''(\mathcal{E}, \mathbf{q}) (\mathcal{E} - \mathcal{E}_0(\mathbf{q}) - (1 - n)\Sigma'(\mathcal{E}, \mathbf{q})) + (1 - n)^2 C'(\mathcal{E}, \mathbf{q}) \Sigma''(\mathcal{E}, \mathbf{q}).
\]

The functions $C'$, $\Sigma'$, and $C''$, $\Sigma''$ are respectively the real and the imaginary parts of the corresponding functions (3.14) and (3.15). They are defined as follows

\[
C(\mathcal{E} + i0, \mathbf{q}) = C'(\mathcal{E}, \mathbf{q}) - iC''(\mathcal{E}, \mathbf{q}), \quad \Sigma(\mathcal{E} + i0, \mathbf{q}) = \Sigma'(\mathcal{E}, \mathbf{q}) - i\Sigma''(\mathcal{E}, \mathbf{q}).
\]

We can see that the expression for the obtained spectral density $g(\mathcal{E})$ does not depend on the magnetization and its fluctuations. It confirms the assumption we have made in the second section to obtain expression (2.16) for the critical temperature.

Let us estimate now the structural fluctuations of magnetization of a magnetic subsystem at low concentration of non-magnetic impurities. To do it we assume that these fluctuations are proportional to the square of concentration of non–magnetic atoms and we shall keep in the numerator of the expression (2.10) for the Green’s function $G_2$ all the terms up to the second order as to the concentration $(1 - n)$ of non–magnetic sites.

Thus we need to sum up the series

\[
\sum_{i=1}^{\infty} \Delta Q_i(\rho + \rho^2)]_\mathbf{q} = \sum_{i=1}^{\infty} [Q_i(\rho + \rho^2)]_\mathbf{q} - \sum_{i=2}^{\infty} [Q_i][\rho^2]_\mathbf{q} = (1 - \sum_{j=2}^{\infty} (\Delta Q_j)\mathbf{q}) (\sum_{i=1}^{\infty} (\Delta Q_i)\mathbf{q} + \sum_{i=2}^{\infty} [Q_i][\rho^2]_\mathbf{q} + o((1 - n)^2))
\]

As we can see from expressions (3.8) and (3.10) the series $\sum_{i=1}^{\infty} (\Delta Q_i)\mathbf{q}$ is of the same order as the fluctuations $\Sigma(\mathcal{E} + i0, \mathbf{q})$ and therefore it is within the made assumptions of the quadratic order with respect to the concentration of non–magnetic impurities. Thus we have

\[
\sum_{i=1}^{\infty} \Delta Q_i(\rho + \rho^2)]_\mathbf{q} \approx \sum_{i=1}^{\infty} (\Delta Q_i)\mathbf{q} + \sum_{i=2}^{\infty} [Q_i][\rho^2]_\mathbf{q} = \sum_{i=2}^{\infty} [Q_i][\rho^2]_\mathbf{q} = (3.27)
\]
It is easy to show that

\[
\sum_{k=1}^{\infty} B_{q,k} \left[ \sum_{k'} \gamma_{q,k'}/q + \sum_{k''} \gamma_{q,k''}/q \right] + \sum_{i=2}^{\infty} N \sum_{k_1, \ldots, k_i} B_{q,k_1} B_{k_2} \ldots B_{k_{i-1}, k_i} \times
\]

\[
\sum_{k_{i+1}} \left( \gamma_{q,k_{i+1}} \right)_{ij} \delta_{k_{i+1}, q} \approx
\]

\[
\sum_{i=1}^{\infty} \sum_{k} |B|_{q,k} \left[ \left( \frac{\xi}{x} \right)^j + \left( \frac{\xi}{x} \right)^{j+1} \right] + \sum_{i=2}^{\infty} N \sum_{k_1, \ldots, k_i} B_{q,k_1} B_{k_2} \ldots B_{k_{i-1}, k_i} \times
\]

\[
\sum_{k_{i+1}} \left( \frac{\xi}{x} \right)^j \sum_{j=2}^{\infty} \left( \frac{\xi}{x} \right)^{j+1} \sum_{\{\lambda\}_{i+1}^{j-1}} \delta \left( q - k_i + \sum_{f=1}^{j-1} (k_{\lambda_f} - k_{\lambda_f-1}) \right) +
\]

\[
\sum_{k_{i+1}} \left( \frac{\xi}{x} \right)^j \sum_{j=2}^{\infty} \left( \frac{\xi}{x} \right)^{j+1} \sum_{\{\lambda\}_{i+1}^{j-1}} \delta \left( q - k_i + \sum_{f=1}^{j-1} (k_{\lambda_f} - k_{\lambda_f-1}) \right) - N \left( \frac{\xi}{x} \right)^j \sum_{k_{i+1}} \delta_{k_{i+1}, q} \right].
\]

It is easy to show that

\[
\sum_{k_{i+1}} \left( \frac{\xi}{x} \right)^j \sum_{j=2}^{\infty} \left( \frac{\xi}{x} \right)^{j+1} \sum_{\{\lambda\}_{i+1}^{j-1}} \delta \left( q - k_i + \sum_{f=1}^{j-1} (k_{\lambda_f} - k_{\lambda_f-1}) \right) =
\]

\[
(3.28)
\]

where \( C^m_n = \binom{n}{m} \) is the binomial coefficient indicating the number of different \( m \)-element subsets of the set \( \{1, \ldots, n\} \). Substituting (3.28) in the expression (3.27) we obtain

\[
\sum_{i=1}^{\infty} |A|_{q,p'=q} \approx
\]

\[
\sum_{i=1}^{\infty} \sum_{k} |B|_{q,k} \left[ \left( \frac{\xi}{x} \right)^j + \left( \frac{\xi}{x} \right)^{j+1} \right] + \sum_{i=2}^{\infty} \sum_{k} |B|_{q,k} \left[ \sum_{j=1}^{i-1} \left( \frac{\xi}{x} \right)^{j+1} \sum_{j=1}^{i-j} \frac{1}{j!} \right].
\]

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Now we substitute in this expression the value of \( \frac{\Delta \sigma^2}{\sigma^2} \) from equation (3.3) and finally we obtain

\[
\sum_{i=1}^{\infty} \left[ \Delta Q_i((\rho + \rho^2)_i) \right] q \approx \left( \frac{\Delta \sigma^2}{\sigma^2} + (1 - n)^2 \right) \sum_{k} B_{q,k} + (1 - n)^2 \sum_{i=2}^{\infty} \sum_{k} [B^i]_{q,k} (-1)^i (2^i - 2) = \tag{3.30}
\]

where we have used the identity

\[
\sum_{j=1}^{i-1} \frac{i!}{j!(i-j)!} = 2^i - 2. \tag{3.31}
\]

Finally we get the following expression for the Green’s function \( \tilde{G}_2 \)

\[
[\tilde{G}_2]_q = 2 \frac{\left( 1 + \sum_{k} B_{q,k} \right) + (1 - n)^2 \sum_{k} [B + (1 + B)^{-1} - (1 + 2B)^{-1}]_{q,k}}{\mathcal{E} - \mathcal{E}_0(q)}, \tag{3.32}
\]

where we have neglected the contribution of disorder to the denominator because of both the terms in the numerator are of the order of the square of the concentration of non–magnetic impurities. It is convenient to distinguish the two parts of this Green’s function as follows

\[
\mathcal{G}_2 = (1 - n)^2 \mathcal{G}_{2a} - \frac{\Delta \sigma^2}{\sigma^2} \mathcal{G}_{2b}, \tag{3.33}
\]

where

\[
[\mathcal{G}_{2a}]_q = 2 \frac{C_a(\mathcal{E}, q)}{\mathcal{E} - \mathcal{E}_0(q),} \quad [\mathcal{G}_{2b}]_q = 2 \frac{1 + C_b(\mathcal{E}, q)}{\mathcal{E} - \mathcal{E}_0(q)} \tag{3.34}
\]

Then we can rewrite the equations for the mean quadratic fluctuations of the magnetization of the magnetic subsystem \((\Delta \sigma)^2\) (2.14) in the following form

\[
\overline{\Delta \sigma^2} = 2(1 - n)^2 \int_{-\infty}^{\infty} \frac{d\mathcal{E}}{e^{\beta(E/h)} - 1} g_{2a}(\mathcal{E}) \left( 1 + 2 \int_{-\infty}^{\infty} \frac{d\mathcal{E}}{e^{\beta(E/h)} - 1} g_{2b}(\mathcal{E}) \right), \tag{3.36}
\]

where

\[
g_{2a}(\mathcal{E}) = -\frac{1}{2\pi N} \text{Sp} \Im \mathcal{G}_{2a}, \quad g_{2b}(\mathcal{E}) = -\frac{1}{2\pi N} \text{Sp} \Im \mathcal{G}_{2b}. \tag{3.37}
\]

Let us consider the low–temperature behaviour of structure fluctuations of the magnetization of the magnetic subsystem \((\Delta \sigma)^2\). Both the integrals in equation (3.36) tend to zero at the temperature tending to zero. Therefore we need only the low–energy behaviour of the spectral density \(g_{2a}\) to obtain the low–temperature asymptotic of the fluctuations \((\Delta \sigma^2)\). In the case of the simple cubic lattice the simple calculations shown in the appendix B yield

\[
g_{2a}(\mathcal{E}) \rightarrow \frac{2}{\pi N} \sum_{q} \delta(\mathcal{E} - \mathcal{E}_0(q)) \tag{3.38}
\]
giving in the three–dimensional case

$$\frac{(\Delta \sigma)^2}{\sigma^2} = 4(1 - n)^2 Z_{3/2}(\beta h) \left( \frac{T}{2\pi nJ} \right)^{3/2},$$

where

$$Z_{\nu}(x) = \sum_{n=1}^{\infty} n^{-\nu} e^{-nx}$$

and $J$ is the exchange integral for the nearest neighbors.

## 4 Conclusions

We have shown that the configurationally averaged Green’s function method is a useful tool for deriving self–consistent equations describing magnetization and its mean quadratic fluctuations caused by disorder. In particular, at low concentration of nonmagnetic impurities we obtain explicit expressions for the spectral densities $g(E)$ and $g_{\Delta}(E)$ giving the value of magnetization $x$ and its quadratic structural fluctuations $(\Delta \sigma)^2$ with respect to the linear concentration of impurities.

We have revealed that the relative quadratic fluctuations of magnetization $(\Delta \sigma)^2/\sigma^2$ could be neglected within the linear as to the concentration of nonmagnetic impurities $1 - n$. They are found to be quadratic over the $1 - n$ and indicate the $T^{3/2}$ behaviour at low temperatures.

The same approach can be applied to describe amorphous and liquid spin systems. It will be the subject of further works.

## A Calculation of the Functions $C$ and $\Sigma$ for the Simple Cubic Lattice

It is easy to show that the matrix element

$$B_{q,k} = \frac{1}{N} A_{q,k} = \frac{1}{N} \sum_{\mathbf{R}} \hat{J}(\mathbf{R}) \left[ (\cos(q\mathbf{R}) - 1) \cos(k\mathbf{R}) + \sin(q\mathbf{R}) \sin(k\mathbf{R}) \right] \frac{E - (1 - \sum_{\mathbf{R}} \hat{J}(\mathbf{R}) \cos(k\mathbf{R}))}{E - \left( 1 - \frac{1}{z} \sum_{l} \cos(kl) \right)}.$$  

For the nearest–neighbour interaction it takes the following form

$$B_{q,k} = \frac{1}{N} \left( \frac{1}{z} \sum_{l} \left[ (\cos(ql) - 1) \cos(kl) + \sin(ql) \sin(kl) \right] \right) \frac{E - (1 - \sum_{l} \cos(kl))}{E - \left( 1 - \frac{1}{z} \sum_{l} \cos(kl) \right)},$$

where $l$ goes over the $z$ nearest neighbours of some site. The fact that the matrix element $B_{q,k}$ is invariant under the transformation $l \rightarrow -l$ allows us to reduce all the sums in expression (A.1) as follows

$$\sum_{l} = \frac{2}{z} \sum'_{l},$$

where a prime denotes that the sum is taken over the $z/2$ nearest neighbours of some site within one half–space. Expression (A.1) can be easily factorized as follows

$$B_{q,k} = \sum_{\mu=1,2}^{'l} \alpha_{l,\mu}(q) \beta_{l,\mu}(E, k),$$

where $l$ goes over the $z$ nearest neighbours of some site.
where
\[
\alpha_{1,1}(k) = \frac{2}{z} (\cos(kl) - 1), \quad \alpha_{1,2}(k) = \frac{2}{z} \sin(kl),
\]
\[
\beta_{1,1}(\mathcal{E}, k) = \frac{\cos(kl)}{N \left[ \mathcal{E} - \left( 1 - \frac{2}{z} \sum \frac{\cos(kl)}{k} \right) \right]}, \quad \beta_{1,2}(\mathcal{E}, k) = \frac{\sin(kl)}{N \left[ \mathcal{E} - \left( 1 - \frac{2}{z} \sum \frac{\cos(kl)}{k} \right) \right]}
\]

Now we can rewrite \( B_{q,k} \) as a matrix product
\[
B_{q,k} = \hat{\alpha}^T (q) \hat{\beta}(\mathcal{E}, k),
\]
where
\[
\hat{\alpha} = \begin{pmatrix} \hat{\alpha}_1 \\ \hat{\alpha}_2 \end{pmatrix} = \begin{pmatrix} \alpha_{1,1} \\ \vdots \\ \alpha_{1,2} \\ \vdots \\ \alpha_{1/2,1} \\ \alpha_{1,2} \\ \vdots \end{pmatrix}, \quad \hat{\beta} = \begin{pmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \end{pmatrix} = \begin{pmatrix} \beta_{1,1} \\ \vdots \\ \beta_{1,2} \end{pmatrix}
\]

After the made transformation the inverse matrix \((1 + B)^{-1}\) can be easily calculated. Indeed
\[
[(1 + B)^{-1}]_{q,k} = \delta_{q,k} + \sum_{i=1}^{\infty} \left[ (-B)^i \right]_{q,k} = \delta_{q,k} - \hat{\alpha}^T (q) \left( 1 + \sum_{i=1}^{\infty} \left(-\hat{\beta}(\mathcal{E}, k')\hat{\alpha}^T(k') \right)^i \right) \hat{\beta}(\mathcal{E}, k) - \delta_{q,k} - \hat{\alpha}^T (q)(1 + \hat{\gamma}(\mathcal{E}))^{-1} \hat{\beta}(\mathcal{E}, k),
\]
where
\[
\hat{\gamma}(\mathcal{E}) = \sum_k \hat{\beta}(\mathcal{E}, k) \hat{\alpha}^T (k).
\]

Thus the problem of calculating the inverse matrix \((1 + B)^{-1}\) of the order \(N\) is reduced to the calculation of inverse matrix \((1 + \hat{\gamma}(\mathcal{E}))^{-1}\) of the order \(z/2\).

Since \(\hat{\alpha}_1\) and \(\hat{\beta}_1\) are even functions of \(k\) and \(\hat{\alpha}_2\) and \(\hat{\beta}_2\) are the odd ones the matrix \(\hat{\gamma}\) has the form
\[
\hat{\gamma}(\mathcal{E}) = \begin{pmatrix} \hat{\gamma}_1(\mathcal{E}) & 0 \\ 0 & \hat{\gamma}_2(\mathcal{E}) \end{pmatrix},
\]
where
\[
\hat{\gamma}_v(\mathcal{E}) = \sum_k \hat{\beta}_v(\mathcal{E}, k) \hat{\alpha}_v^T (k).
\]

Now we can easily express the functions \(C\) defined in [3.10], [3.33] in terms of the matrices \(\hat{\alpha}, \hat{\beta}\) and \(\hat{\gamma}\)
\[
C(\mathcal{E}, q) = \sum_k [B(1 + B)^{-1}]_{q,k} = \hat{\alpha}^T (q)(1 + \hat{\gamma}(\mathcal{E}))^{-1} \hat{\beta}(\mathcal{E}),
\]
\[
C_\alpha(\mathcal{E}, q) = \sum_k [B + (1 + B)^{-1} - (1 + 2B)^{-1}]_{q,k} = \hat{\alpha}^T (q) \left[ 1 + 2(1 + 2\hat{\gamma}(\mathcal{E}))^{-1} - (1 + \hat{\gamma}(\mathcal{E}))^{-1} \right] \hat{\beta}(\mathcal{E}),
\]
\[
C_\beta(\mathcal{E}, q) = \sum_k B_{q,k} = \hat{\alpha}^T (q) \hat{\beta}(\mathcal{E}),
\]

where
where
\[ \hat{B}(\mathcal{E}) = \sum_k \hat{\beta}(\mathcal{E}, k). \] (A.11)

To obtain a similar expression for the function \( \Sigma \) we rewrite the matrix \( A \) in a similar way as the \( B \):
\[ A_{q,k} = \hat{\alpha}^T(q) \hat{\eta}(k), \]
where
\[
\hat{\eta} = \begin{pmatrix} \hat{\eta}_1 \\ \hat{\eta}_2 \end{pmatrix} = \begin{pmatrix} \eta_{1,1} \\ \vdots \\ \eta_{n/2,1} \\ \eta_{1,2} \\ \vdots \\ \eta_{n/2,2} \end{pmatrix}, \quad \eta_{1,1}(k) = \cos(kl) \quad \eta_{1,2}(k) = \sin(kl). \quad (A.12)
\]

Thus we can rewrite the expression for the function \( \Sigma \) as follows
\[ \Sigma(\mathcal{E}, q) = \left[ B_1 + B_2 \right]_{q,q} = \hat{\alpha}^T(q)(1 + \hat{\gamma}(\mathcal{E}))^{-1} \hat{\eta}(q) = \hat{\alpha}^T(q) \hat{\eta}(q) - \hat{\alpha}^T(q)(1 + \hat{\gamma}(\mathcal{E}))^{-1} \hat{\eta}(q). \quad (A.13)\]

The calculation of the inverse matrix \((1 + \hat{\gamma}(\mathcal{E}))^{-1}\) can be easily carried out for any simple lattice. Let us consider as an example the \( d \)-dimensional simple cubic lattice. Then we have
\[ (kl) = k_i a, \quad i = 1, \ldots, d, \]
where \( a \) is a lattice constant. The matrix \( \hat{\gamma} \) takes the form
\[
\hat{\gamma} = \begin{pmatrix} \phi & \chi & \cdots & \chi \\ \chi & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \chi \\ \chi & \cdots & \chi & \phi \\ \psi & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \psi \end{pmatrix}. \quad (A.14)
\]

All the diagonal elements of the matrix \( \hat{\gamma}_1 \) read
\[
\phi = \frac{1}{d} \frac{1}{N} \sum_k \frac{\cos^2(k_1 a) - \cos(k_1 a)}{\mathcal{E} - \mathcal{E}_{\alpha}(k)} = \frac{1}{d} \left( I_{\mathcal{E}}^d(\mathcal{E}) - I_{\mathcal{E}_{\alpha}}^d(\mathcal{E}) \right), \quad (A.15)
\]
where as the off-diagonal elements read
\[
\chi = \frac{1}{d} \frac{1}{N} \sum_k \frac{\cos(k_1 a) \cos(k_2 a) - \cos(k_1 a)}{\mathcal{E} - \mathcal{E}_{\alpha}^d(\mathcal{E})} = \frac{1}{d} \left( I_{\mathcal{E}_{\alpha}}^d(\mathcal{E}) - I_{\mathcal{E}_{\alpha}}^d(\mathcal{E}) \right). \quad (A.16)
\]

The matrix \( \hat{\gamma}_2 = \psi \hat{1} \), where
\[
\psi = \frac{1}{d} \frac{1}{N} \sum_k \frac{\sin^2(k_1 a)}{\mathcal{E} - \mathcal{E}_{\alpha}^d(\mathcal{E})} = \frac{1}{d} I_{\mathcal{E}_{\alpha}}^d(\mathcal{E}). \quad (A.17)
\]

Here
\[
\mathcal{E}_{\alpha}^d(\mathcal{E}) = 1 - \frac{1}{d} \sum_{i=1}^d \cos(k_i a) \quad (A.18)
\]
is a dimensionless energy of spin excitations of the non–dilute simple cubic ferromagnet and we have introduced the following notation

\[
I_c^d(\mathcal{E}) = \frac{1}{N} \sum_k \frac{\cos^2(k_1 a)}{\mathcal{E} - \mathcal{E}^0_c(k)}, \quad I_c^d(\mathcal{E}) = \frac{1}{N} \sum_k \frac{\cos(k_1 a)}{\mathcal{E} - \mathcal{E}^0_c(k)},
\]

\[
I_e^d(\mathcal{E}) = \frac{1}{N} \sum_k \frac{\cos(k_1 a) \cos(k_2 a)}{\mathcal{E} - \mathcal{E}^0_e(k)}, \quad I_s^d(\mathcal{E}) = \frac{1}{N} \sum_k \frac{\sin^2(k_1 a)}{\mathcal{E} - \mathcal{E}^0_s(k)}.
\]

Let us note that the sum \(\sum_k \hat{\beta}\) that appeared in the expressions for the functions \(C\) can be rewritten as

\[
\sum_k \hat{\beta}_1(\mathcal{E}, k) = I_c^d(\mathcal{E}) \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}, \quad \sum_k \hat{\beta}_2(\mathcal{E}, k) = 0. \tag{A.20}
\]

It can be easily verified directly that

\[
(1 + \hat{\gamma}_1)^{-1} = \frac{1/d}{1 + \phi + (d-1)\chi} \begin{pmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{pmatrix} + \frac{1/d}{1 + \phi - \chi} \begin{pmatrix} d - 1 & -1 & \cdots & -1 \\ -1 & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ -1 & \cdots & -1 & d - 1 \end{pmatrix}. \tag{A.21}
\]

Now we can rewrite the expressions for the functions \(C\) as follows

\[
C(\mathcal{E}, q) = \hat{\alpha}_1^T(q)(1 + \hat{\gamma}_1(\mathcal{E}))^{-1} \hat{B}_1(\mathcal{E}, k) = \frac{-I_c^d(\mathcal{E})\mathcal{E}^0_c(q)}{1 + \phi + (d-1)\chi} \frac{\mathcal{E}^0_c(q)}{\mathcal{E} - \frac{1}{\mathcal{E}_c(q)}}. \tag{A.22}
\]

\[
C_a(\mathcal{E}, q) = \hat{\alpha}_1^T(q) \left[ 1 + 2(1 + 2\hat{\gamma}_1(\mathcal{E}))^{-1} - (1 + \hat{\gamma}_1(\mathcal{E}))^{-1} \right] \hat{B}_1(\mathcal{E}) = \frac{-I_c^d(\mathcal{E})\mathcal{E}^0_c(q)}{2\phi + 2(d-1)\chi} + \frac{I_c^d(\mathcal{E})\mathcal{E}^0_c(q)}{1 + \phi + (d-1)\chi} = \mathcal{E}^0_c(q) \left[ -I_c^d(\mathcal{E}) + \frac{1}{\mathcal{E} - \frac{1}{\mathcal{E}_c(q)}} - \frac{1}{\mathcal{E} - \frac{1}{\mathcal{E}_c(q)}} \right], \tag{A.23}
\]

\[
C_b(\mathcal{E}, q) = \hat{\alpha}_1^T(q) \sum_k \hat{\beta}_1(\mathcal{E}, k) - I_c^d(\mathcal{E})\mathcal{E}^0_c(q), \tag{A.24}
\]

where we have used the fact that

\[
0 = \frac{1}{N} \sum_k \frac{1}{d} \sum_i \cos(k_i a) = \frac{1}{N} \sum_k \frac{1}{d} \sum_i \cos(k_i a) \frac{\mathcal{E} - 1 + \frac{1}{d} \sum_j \cos(k_j a)}{(\mathcal{E} - 1)I_c^d(\mathcal{E}) + \frac{1/d}{I_c^d(\mathcal{E})} + \frac{d-1/d}{I_c^d(\mathcal{E})}} = \frac{(\mathcal{E} - 1)I_c^d(\mathcal{E}) + \frac{1/d}{I_c^d(\mathcal{E})} + \frac{d-1/d}{I_c^d(\mathcal{E})}} \quad \tag{A.25}
\]

and

\[
\phi + (d-1)\chi = \frac{1}{d}I_c^d(\mathcal{E}) + \frac{d-1}{d}I_c^d(\mathcal{E}) - I_c^d(\mathcal{E}) = -\mathcal{E}I_c^d(\mathcal{E}) \tag{A.26}
\]

We can obtain the expression for the function \(\Sigma\) in a similar way.

\[
\Sigma(\mathcal{E}, q) = \hat{\alpha}_1^T(q)(1 + \hat{\gamma}(\mathcal{E}))^{-1}\hat{\gamma}(\mathcal{E}))\hat{\eta}(q) = \hat{\alpha}_1^T(q)\hat{\eta}_1(q) - \hat{\alpha}_1^T(q)(1 + \hat{\gamma}(\mathcal{E}))^{-1}\hat{\eta}_1(q) + \frac{\psi}{1 + \psi}\hat{\alpha}_2^T(q)\hat{\eta}_2(q) = \]

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Let us calculate the function 

\[ \frac{1}{d} \sum_i (\cos(k_i a) - 1) \cos(k_i a) + \frac{I_{c2}^d(\mathcal{E})}{d + I_{cc}^d(\mathcal{E})} \frac{1}{d} \sum_i \sin^2(k_i a) - \]

\[ \frac{1}{1 - \mathcal{E} I_c^d(\mathcal{E})} \frac{1}{d^2} \sum_{i,j} (\cos(k_i a) - 1) \cos(k_j a) - \]

\[ \frac{1}{d + I_{cc}^d(\mathcal{E}) - I_{cc}^d(\mathcal{E})} \left( \sum_i (\cos(k_i a) - 1) \cos(k_i a) - \frac{1}{d} \sum_{i,j} (\cos(k_i a) - 1) \cos(k_j a) \right) = \]

\[ \mathcal{E}_0(k) - 2 \mathcal{E}_1(k) + 2 \frac{I_{c2}^d(\mathcal{E})}{d + I_{c2}^d(\mathcal{E})} \mathcal{E}_1(k) + \]

\[ \frac{1}{1 - \mathcal{E} I_c^d(\mathcal{E})} (\mathcal{E}_0(k) - \mathcal{E}_0^2(k)) + \frac{d}{d + I_{cc}^d(\mathcal{E}) - I_{cc}^d(\mathcal{E})} (2 \mathcal{E}_1(k) - 2 \mathcal{E}_0(k) + \mathcal{E}_0^2(k)), \]  \hspace{1cm} (A.27)

where

\[ \mathcal{E}_1(k) = \frac{1}{2d} \sum_i \sin^2(k_i a). \]  \hspace{1cm} (A.28)

Let us consider the long–wave solutions of equation (3.16) for the spin excitation spectrum. Taking into account that

\[ \mathcal{E}_0(k) = \frac{a^2}{2d} k^2 + o(k^2) \quad \text{and} \quad \mathcal{E}_1(k) = \frac{a^2}{2d} k^2 + o(k^2) \]  \hspace{1cm} (A.29)

we can easily find that

\[ \Sigma(\mathcal{E}, \mathbf{q}) = -2 \frac{a^2}{2d} \frac{I_{c2}^d(\mathbf{q})}{1 - I_{c2}^d(\mathbf{q})} k^2 + o(k^2), \]  \hspace{1cm} (A.30)

where

\[ I_{c2}^d(d) = -\frac{1}{d} I_{c2}^d(0) = \frac{1}{N} \sum_k \frac{\sin^2(k_1 a)}{\sum_i (1 - \cos(k_i a))}. \]  \hspace{1cm} (A.31)

## B Calculation of the Spectral Density \( g_{2a} \) for the Simple Cubic Lattice

Let us calculate the function

\[ g_{2a}(\mathcal{E}) \equiv -\frac{1}{2\pi N} \text{Sp} \overline{\mathcal{G}_{2a}} \]  \hspace{1cm} (B.1)

we need to obtain the low–temperature behaviour of the structural quadratic fluctuations of magnetization \( \langle \Delta \sigma \rangle^2 \). Using the result of the previous section we get the \( d \)-dimensional \((sc)\) lattice

\[ g_{2a}(\mathcal{E}) = -\frac{1}{2\pi N} \text{Sp} \overline{\mathcal{G}_{2a}} = -\frac{1}{\pi N} \sum_{\mathbf{q}} \frac{C_{2a}(\mathcal{E}, \mathbf{q})}{\mathcal{E} - \mathcal{E}_0(\mathbf{q})} \bigg|_{\mathcal{E}+i0} = \]

\[ -\frac{1}{\pi N} \sum_{\mathbf{q}} \frac{\mathcal{E}_0^sc(\mathbf{q})}{\mathcal{E} - \mathcal{E}_0^sc(\mathbf{q})} \left[ -I_{c}^d(\mathcal{E}) + \frac{1}{\mathcal{E} - \frac{1}{2\mathcal{E}_c(\mathcal{E})}} - \frac{1}{\mathcal{E} - \frac{1}{I_{cc}^d(\mathcal{E})}} \right] \bigg|_{\mathcal{E}+i0} = \]

\[ \frac{1}{\pi} \sum_{\mathcal{E}} U_\mathcal{E} \left[ -I_{c}^d(\mathcal{E}) + \frac{1}{\mathcal{E} - \frac{1}{2\mathcal{E}}} - \frac{1}{\mathcal{E} - \mathcal{V}_\mathcal{E}} \right] \bigg|_{\mathcal{E}+i0}. \]

Here

\[ U_\mathcal{E} = -\frac{1}{N} \sum_{\mathbf{q}} \frac{\mathcal{E}_0^sc(\mathbf{q})}{\mathcal{E} - \mathcal{E}_0^sc(\mathbf{q})} = I_{c2}^d(\mathcal{E}) - I_{c1}^d(\mathcal{E}), \quad I_{c1}^d(\mathcal{E}) = \frac{1}{N} \sum_k \frac{1}{\mathcal{E} - \mathcal{E}_0^sc(\mathbf{k})}, \quad \mathcal{V}_\mathcal{E} = \frac{1}{I_{cc}^d(\mathcal{E})}. \]  \hspace{1cm} (B.3)
Simple calculations give us the following expression for the spectral density

\[ g_{2o}(\mathcal{E}) = \frac{1}{\pi} \left\{ U_\mathcal{E} \left[ I_\mathcal{E}^{d''}(\mathcal{E}) + \frac{2V''_\mathcal{E}}{(2\mathcal{E} - V'_\mathcal{E})^2 + (V''_\mathcal{E})^2} - \frac{V''_\mathcal{E}}{(\mathcal{E} - V'_\mathcal{E})^2 + (V''_\mathcal{E})^2} \right] \right\} - U'_\mathcal{E} \left[ -I_\mathcal{E}'(\mathcal{E}) + \frac{4\mathcal{E} - 2V'_\mathcal{E}}{(2\mathcal{E} - V'_\mathcal{E})^2 + (V''_\mathcal{E})^2} - \frac{\mathcal{E} - V'_\mathcal{E}}{(\mathcal{E} - V'_\mathcal{E})^2 + (V''_\mathcal{E})^2} \right], \]

where

\[ U_{\mathcal{E}+i\delta} = U_\mathcal{E}' - iU_\mathcal{E}'' , \quad V_\mathcal{E} = \frac{1}{I_\mathcal{E}'(\mathcal{E})}, \quad V_{\mathcal{E}+i\delta} = \frac{1}{I_\mathcal{E}'(\mathcal{E}) - iI_\mathcal{E}''(\mathcal{E})} = V_\mathcal{E}' + iV_\mathcal{E}'' . \]  

Let us consider an asymptotic behaviour of the spectral density \( g_{2o}(\mathcal{E}) \) at small \( \mathcal{E} \).

\[ U_\mathcal{E}' = -\frac{\mathcal{P}}{N} \sum_k \frac{\mathcal{E}_0^{sc}(k)}{\mathcal{E} - \mathcal{E}_0^{sc}(k)} = 1 - \mathcal{E} \frac{\mathcal{P}}{N} \sum_k \frac{1}{\mathcal{E} - \mathcal{E}_0^{sc}(k)} \to 1 , \]

\[ U_\mathcal{E}'' = -\frac{\pi}{N} \sum_k \mathcal{E}_0^{sc}(k)\delta(\mathcal{E} - \mathcal{E}_0^{sc}(k)) = -\pi\mathcal{E}g_0(\mathcal{E}) , \]

\[ I_\mathcal{E}'(\mathcal{E}) = \frac{\mathcal{P}}{N} \sum_k \frac{1}{\mathcal{E} - \mathcal{E}_0^{sc}(k)} \]

\[ I_\mathcal{E}''(\mathcal{E}) = \frac{\pi}{N} \sum_k (1 - \mathcal{E}_0^{sc}(k))\delta(\mathcal{E} - \mathcal{E}_0^{sc}(k)) = \pi(1 - \mathcal{E})g_0(\mathcal{E}) \to \pi g_0(\mathcal{E}) , \]

\[ V_\mathcal{E}' = \frac{I_\mathcal{E}''(\mathcal{E})}{(I_\mathcal{E}'(\mathcal{E}))^2 + (I_\mathcal{E}''(\mathcal{E}))^2} , \quad V_\mathcal{E}'' = \frac{I_\mathcal{E}''(\mathcal{E})}{(I_\mathcal{E}'(\mathcal{E}))^2 + (I_\mathcal{E}''(\mathcal{E}))^2} . \]

Here

\[ g_0(\mathcal{E}) = \frac{1}{N} \sum_k \delta(\mathcal{E} - \mathcal{E}_0^{sc}(k)) \]

is the density of states of a non–dilute crystal. Finally we get

\[ g_{2o}(\mathcal{E}) \to \frac{1}{\mathcal{E} \to 0} \pi^{\frac{1}{2}} \left( U_\mathcal{E}'' I_\mathcal{E}'(\mathcal{E}) + I_\mathcal{E}''(\mathcal{E}) U_\mathcal{E}' + \frac{U_\mathcal{E}'' V_\mathcal{E}'}{(V_\mathcal{E}')^2 + (V_\mathcal{E}'')^2} - \frac{2}{\pi} \left( U_\mathcal{E}'' I_\mathcal{E}'(\mathcal{E}) + I_\mathcal{E}''(\mathcal{E}) U_\mathcal{E}' \right) \right) \to 2g_0(\mathcal{E}) . \]  

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