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The internal energies of Heisenberg magnetic systems

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ABSTRACT

The internal energies, including transverse and longitudinal parts, of quantum Heisenberg systems for arbitrary spin S are investigated by the double-time Green's function method. The expressions for ferromagnetic (FM) and antiferromagnetic (AFM) systems are derived when one-component of magnetization is considered with the higher order longitudinal correlation functions being carefully treated. An unexpected result is that around the order–disorder transition points the neighboring spins in a FM (AFM) system are more likely longitudinally antiparallel (parallel) than parallel (antiparallel) to each other for $S \leq 3/2$ in spite of the FM (AFM) exchange between the spins. This is attributed to the strong quantum fluctuation of the systems with small S values. We also present the expressions of the internal energies of FM systems when the three-component of magnetizations are considered.

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1. Introduction

The quantum Heisenberg model has been studied enduringly. The double-time Green's function method [1], being applicable in the whole temperature range, has been employed to solve the model over half a century [2–19]. For a long time, the magnetization along the z direction was calculated, with the assumption that the components other than this direction were zero [2–11]. Since 2000, a skill has been developed to calculate all the three components of the magnetization [12–19]. In calculation of the magnetizations, the equation of motion (EOM) of the Green's functions is applied, and the higher-order Green's functions are usually decoupled to the lower-order ones in terms of the well-known Tyablikov decoupling [2], also called the random phase approximation (RPA).

It is generally believed that evaluation of the magnetizations under the RPA is quite reasonable. However, the internal energies obtained up to now have not been satisfactory. The internal energies of antiferromagnetic (AFM) lattices at temperature close to zero was discussed [3]. A viewpoint was that it was better to go beyond the RPA in order to achieve satisfactory internal energies [18]. That is to say, higher-order Green's functions have to be solved. However, it is very difficult to do so. There has not been much work [20–26] attempting to solve the higher-order Green's functions and they were usually limited to the low-dimensional lattices and the lowest spin quantum number $S=1/2$. Even for the low-dimensional systems, it was difficult to deal with the cases

with higher spin quantum numbers. The only instance of dealing with the higher S values was confined in finite lattice site systems [25]. A remarkable progress was the calculation of the internal energies of ferromagnetic (FM) lattices above the Curie point by means of the higher-order Green's functions [27]. There was one common feature in the work presented in Refs. [20–27]: the higher-order Green's functions were constructed in the cases where the magnetization was zero.

To sum up, the evaluation of the internal energy of the Heisenberg systems when the magnetization was not zero by means of the Green's function method has seldom been there to see. We believe that under the RPA, it is possible to obtain as good as possible expressions for the internal energy applicable to any S value for nonzero magnetization.

The internal energy of a Heisenberg magnetic system mainly includes two parts, the transverse correlation energy (TCE) and longitudinal correlation energy (LCE), as defined in Eqs. (3) and (4) below. The former is easily calculated by means of the well-known spectral theorem without any further approximation [5,18,28]. Hereafter, when no further approximation is made in giving an expression of the energy, we say the expression is precise. In this sense, the expression of the TCE is precise. The LCE, however, can be dealt with precisely only in the case of $S=1/2$ and 1 [18,28,29]. For higher S values, the treatment of this part is troublesome. At first thought, the following approximation can be taken [5]:

$$\langle S_i^z S_j^z \rangle \approx \langle S_i^z \rangle \langle S_j^z \rangle, \quad i \neq j \quad (1)$$

where the subscripts label the lattice sites. In previous work, we also employed this approximation [30]. However, this approximation is obviously too rough. A good approximation of the longitudinal correlation function valid for any S value and temperature

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is still desirable. In this paper, we will present satisfactory expressions of the internal energies for some magnetic systems.

2. One-component magnetization: ferromagnetic systems

The Hamiltonian reads

$$H = -\frac{1}{2}J\sum_{ij}S_i^-S_j^+ - \frac{1}{2}J\sum_{ij}S_i^zS_j^z - K_z\sum_i(S_i^z)^2 - b_z\sum_iS_i^z \quad (2)$$

Throughout this paper, we consider the nearest neighbor exchanges, and the lower case English letters label lattice sites. In Eq. (2), $J > 0$. The first two terms reflect the transverse and longitudinal correlations between the neighboring magnetic moments, respectively. At finite temperature, any moment has an instant orientation along the directions other than the z direction due to its thermomotion, which is embodied in the transverse correlation function. The third term is the single-ion anisotropy along the z direction that forces the spontaneous magnetization along this direction. The fourth term is the Zeeman energy when an external magnetic field b_z along the z direction is applied. For the sake of convenience, we hereafter denote $S_p = S(S+1)$.

The internal energy is defined as the statistical average of the Hamiltonian per site, $U_{IN} = \langle H \rangle / N$, where N is the total site number in the system. Thus, the first two terms of the internal energy are written as

$$U_{TC} = -\frac{1}{2}J\sum_j \langle S_0^- S_j^+ \rangle \quad (3)$$

and

$$U_{LC} = -\frac{1}{2}J\sum_j \langle S_0^z S_j^z \rangle \quad (4)$$

and are termed as TCE and LCE, respectively. The subscript 0 means the origin and the summations are taken over its nearest neighbors.

As has been mentioned, the first rough approximation made for the LCE was Eq. (1). This was plausible when checking its value at two special temperatures, zero and the Curie point. At $T=0$, the internal energy, with the absence of the external field and anisotropy, is

$$U_{IN}(T=0) = U_{LC}(T=0) = -\frac{1}{2}J(0)S^2 \quad (5)$$

where we have defined $J(0) = c_1 J$ with the c_1 being the nearest neighbor number. The quantity $J(0)$ is in fact the case of taking the wave vector $\mathbf{k}=0$ in the Fourier component of the exchange parameter $J(\mathbf{k}) = J\sum_{\mathbf{a}} e^{i\mathbf{k}\cdot\mathbf{a}}$, where the summation is over the nearest neighbors of the origin.

Eq. (5) is the rigorous ground-state energy of a FM system. At the Curie point T_C , the spontaneous magnetization becomes zero. So it seems plausible that $U_{LC}(T=T_C) = 0$. However, the analysis is not reliable. At $T=0$, Eq. (5) happens to be correct for FM lattices because the spontaneous magnetization is along the z direction and there is no transverse correlation between neighboring spins. In the case of an AFM system, even at zero temperature, the neighboring spins are not rigorously antiparallel to each other, and there is the transverse correlation effect. At this point Eq. (1) exposes its drawback. At order-disorder transition temperature such as T_C (T_N) for FM (AFM) lattices, although the spontaneous magnetization becomes zero, the LCE may not be zero due to the existence of the short-range correlation effect [27,31–33]. Hence, a smart treatment of this energy is required. In the following, we make use of the Green's function method to derive the expressions of the energies.

The double-time Green's function is defined as $G_{ij}(t, t') = \langle\langle A_i(t); B_j(t') \rangle\rangle$ where the two operators in the present section are chosen as $A = S^+$ and $B(u) = e^{uS^z} S^-$.

Note that there is a parameter u in the operator B . In applying the EOM method, the first job is to reckon the commutator of an operator S_i^+ and the Hamiltonian:

$$[S_i^+, H] = -J\sum_j (S_i^z S_j^+ - S_i^+ S_j^z) + K_z(S_i^z S_i^+ + S_i^+ S_i^z) + b_z S_i^+ \quad (6)$$

Then the higher order Green's functions are decoupled by the RPA. Subsequently, the Fourier component of $G_{ij}(t, t')$, denoted as $g(\mathbf{k}, \omega)$, is solved

$$\mathbf{g}(\mathbf{k}, \omega) = \frac{[A, B(u)]}{\omega - \omega(\mathbf{k})} \quad (7)$$

The dispersion relation is $\omega(\mathbf{k}) = (|J(0)| + K_z C)(1 - \gamma_{\mathbf{k}C})\langle S^z \rangle + b_z$, where the notation $\gamma_{\mathbf{k}}$ is defined as $\gamma_{\mathbf{k}C} = J(\mathbf{k}) / (|J(0)| + K_z C)$. The coefficient C came from the Anderson–Callen version of the decoupling concerning the single-ion term [6].

By means of the well-known spectral theorem, we obtain the evaluation of the correlation function of the two operators:

$$\langle B_{\mathbf{m}}(u, t') A_{\mathbf{l}}(t) \rangle = \langle [A, B(u)] \rangle \sum_{\mathbf{k}} \frac{e^{-i\omega(\mathbf{k})(t-t')}}{e^{\beta\omega(\mathbf{k})} - 1} e^{-i\mathbf{k}(\mathbf{l}-\mathbf{m})}, \quad (8)$$

where $\beta = 1/T$, the inverse of temperature. We have set Boltzman constant $k_B = 1$. In Eq. (8), let $t = t'$ and $\mathbf{l} = \mathbf{m}$, then under the RPA, the expression of the magnetization can be solved from an ordinary differential equation of the second order [4,19,28,34,35]:

$$\langle S^z \rangle = \frac{(\Phi + S)\Phi^{2S+1} - (\Phi - S)(\Phi + 1)^{2S+1}}{(\Phi + 1)^{2S+1} - \Phi^{2S+1}}, \quad (9)$$

where

$$\Phi = \sum_{\mathbf{k}} \frac{1}{e^{\beta\omega(\mathbf{k})} - 1} \quad (10)$$

From Eqs. (9) and (10), $\langle S^z \rangle$ is computed iteratively. Consequently, the following three correlations can be evaluated:

$$\langle (S^z)^2 \rangle = S_p - (1 + 2\Phi)\langle S^z \rangle, \quad (11)$$

$$\langle (S^z)^3 \rangle = [(1 + 2\Phi)[S_p - 3\langle (S^z)^2 \rangle] + (2S_p - 1)\langle S^z \rangle] / 2 \quad (12)$$

and

$$\langle (S^z)^4 \rangle = S_p^2 - \langle (S^z)^2 \rangle - 2(1 + 2\Phi)\langle (S^z)^3 \rangle \quad (13)$$

From Eq. (8) two formulas can be derived. Note the definition of the operators A and B . Substituting them into (8), letting $t = t'$, taking derivative n times with respect to the parameter u , letting $u=0$ and then summing over the nearest neighbors of site \mathbf{m} , we obtain

$$J\sum_j \langle (S_{\mathbf{m}}^z)^n S_{\mathbf{m}}^- S_j^+ \rangle = \Phi_a \langle [S^+, (S^z)^n S^-] \rangle, \quad (14)$$

where we have defined

$$\Phi_a = \frac{1}{N} \sum_{\mathbf{k}} \frac{J(\mathbf{k})}{e^{\beta\omega(\mathbf{k})} - 1} \quad (15)$$

Now let us take derivative with respect to time t :

$$\langle B_{\mathbf{m}}(u, t') [A_{\mathbf{l}}(t), H] \rangle = \langle [A, B(u)] \rangle \sum_{\mathbf{k}} \frac{\omega(\mathbf{k}) e^{-i\omega(\mathbf{k})(t-t')}}{e^{\beta\omega(\mathbf{k})} - 1} e^{-i\mathbf{k}(\mathbf{l}-\mathbf{m})} \quad (16)$$

Letting $t = t'$, taking derivative n times with respect to the parameter u and then letting $u=0$, we achieve

$$\langle (S_0^z)^n S_0^- [S_0^+, H] \rangle = \Phi_b \langle [S^+, (S^z)^n S^-] \rangle, \quad (17)$$

where

$$\Phi_b = \frac{1}{N} \sum_{\mathbf{k}} \frac{\omega(\mathbf{k})}{e^{\beta\omega(\mathbf{k})} - 1} \quad (18)$$

Eqs. (14) and (17) are quite useful for calculation of the LCEs.

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