Quantum Heisenberg model with long-range ferromagnetic interactions: A Green's function approach

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A Green-function method is employed within a random phase approximation to study the one-dimensional quantum Heisenberg model with long-range ferromagnetic interaction proportional to r^{-p}. We have shown that for $1<p<2$ there exists a phase transition at finite temperatures and estimate its critical temperature.

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I. INTRODUCTION

The investigation of low-dimensional magnetism is an important branch of modern solid state physics. Experimental interest in this problem is connected with the magnetic properties of copper oxide high-temperature superconductors, organic compounds, films, and surfaces. Recently, low-dimensional magnetic systems have received a great deal of attention. Several theoretical techniques have been employed to understand the magnetic properties of these systems.

High-temperature series expansions combined with the Padé approximant method,[1] spin wave theory,[2–6] Monte Carlo simulations,[7,8] renormalization group,[9,10] and the Green's function formalism[11,12] are some of the methods used in these studies. Recently the method of double-time spin Green's function has been extensively used in the literature for the investigation of the ferromagnetic and antiferromagnetic Heisenberg model with nearest-neighbor interaction. The method is valid even in dimension less than three. Yablonskiy[12] used it to study the static properties of the one- and two-dimensional quantum system described by the Heisenberg model. The theory predicts correctly the absence of long-range order in finite temperature, produced an exponentially divergent correlation length when the temperature approaches absolute zero, and gave good qualitative agreement over the wide temperature range with both the modified spin-wave theory of Takahashi[13] and the Schwinger bosonic and fermionic representation of Arovas and Auerbach.[14] Also the method combined with the so-called random phase approximation (RPA) has been extended successfully to study the charge and spin correlation functions in the one-dimensional Hubbard model.[15] In this paper, we show that, with the aid of Green's function formalism, we are able to show that there exists a phase transition from ferromagnetic to paramagnetic phase for some ferromagnetic low-dimensional system with long-range interactions ($d=1,2$) described by the Heisenberg model.

II. CALCULATIONS

We consider the following Hamiltonian of a one-dimensional Heisenberg ferromagnetic model:

$$H=\sum_{\langle nm\rangle} J_{n,m}\vec{S}_n\vec{S}_m \tag{1}$$

where the summation is over the nearest-neighbor pairs of $\frac{1}{2}$ spins, $\langle nm\rangle$ denotes a pair of nearest-neighbor sites and $J_{n,m}$ is the exchange coupling between neighboring spins with

$$J_{n,m}=J|n-m|^{-p}=Jr^{-p}. \tag{2}$$

We consider the Green function

$$G_{g,l}\equiv -i\theta(t)\langle\langle S_g^+(t);S_l^-\rangle\rangle. \tag{3}$$

The Fourier transform of this Green function, satisfies the equation of motion

$$EG_{g,l}(E)=\frac{1}{2\pi}\langle[S_g^+,S_l^-]\rangle+\langle\langle[[S_g^+(t),H];S_l^-(0)]\rangle\rangle_E, \tag{4}$$

where g and l are two lattice sites and $G_{g,l}(E)$ is the Fourier transform of the Green's function $\langle\langle S_g^+(t),S_l^-\rangle\rangle$.

In order to solve the system of equation generated by Eq. (4), we need to break the chain of the Green's functions. In this paper we consider the simplest decoupling scheme, the random phase approximation (RPA), where the longitudinal and transversal components of the spin operators at different sites of the lattice are uncorrelated,[16] that is,

$$\langle\langle S_g^zS_i^+;S_l^-\rangle\rangle=\langle S_g^z\rangle\langle\langle S_i^+;S_l^-\rangle\rangle. \tag{5}$$

Taking into account the translation symmetry of the lattice we can write that

$$G_{g,l}(E)=\frac{1}{N}\sum_k G_k(E)\exp[ik(g-l)], \tag{6}$$

where the summation is over the set of k vectors inside the first Brillouin zone. In this way we find that

$$G_k(E)=\frac{\langle S^z\rangle}{\pi}\frac{1}{[E-E_k]}, \tag{7}$$

where

$$E_k=2\langle S^z\rangle[J_0-J_k] \tag{8}$$

is the magnon energy spectrum, and J_k is the Fourier transform of the exchange integral defined by

$$J_k=\sum_{n,m} J_{n,m}\exp ik(n-m) \tag{9}$$

with the help of the spectral density function,[16] defined as

$$\Delta(E)=i\lim_{\epsilon\to 0}\frac{G(E+i\epsilon)-G(E-i\epsilon)}{\exp\left(\frac{E}{k_BT}\right)-1} \tag{10}$$

we can find the equilibrium correlation function, through

$$\langle S^-S^+\rangle=\int_{-\infty}^{+\infty}\Delta(E)\exp\left(\frac{E}{k_BT}\right)dE. \tag{11}$$

As for spin $S=\frac{1}{2}$ we can write that

$$\langle S^z\rangle=\frac{1}{2}-\langle S^-S^+\rangle, \tag{12}$$

and using the fact that

$$\lim_{\epsilon\to 0^+}\left[\frac{1}{E+i\epsilon-E_k}-\frac{1}{E-i\epsilon-E_k}\right]=-2\pi i\,\delta(E-E_k) \tag{13}$$

we finally arrive at the following expression for the magnetization:

$$\frac{1}{2\langle S^z\rangle}=\frac{1}{N}\sum_k \coth\left(\frac{E_k}{2k_BT}\right). \tag{14}$$

By replacing the summation by an integral over the one-dimensional Brillouin zone, we can write that

$$\frac{1}{2\langle S^z\rangle}=\frac{v}{2\pi}\int_{ZB}\coth\left(\frac{E_k}{2k_BT}\right)dk, \tag{15}$$

where v is the volume of the unitary cell. This equation gives us the magnetization as a function of the temperature and can be solved self-consistently. On the other hand, near the critical temperature, where $\langle S^z\rangle$ goes to zero, we expand the argument into the integral, in Eq. (15), because it is very small. In this case, it is easy to show that

$$\langle S^z\rangle=\left[\frac{3k_BT}{A}\left[1-\frac{T}{T_c}\right]\right]^{1/2}, \tag{16}$$

where

$$\frac{1}{T_c}=\frac{v}{2\pi}\int_{ZB}\frac{dk}{[J_0-J_k]} \tag{17}$$

and

$$A=\frac{1}{zJ}\frac{v}{2\pi}\int_{ZB}[J_0-J_k]dk, \tag{18}$$

with

$$J_0-J_k=zJ\sum_{n=1}^{\infty} n^{-p}[1-\cos(kn)]. \tag{19}$$

For small k and $1<p<3$ we have from[13]

$$2\sum_{n=1}^{\infty} n^{-p}[1-\cos(kn)]=w(p)k^{p-1}, \tag{20}$$

where $w(p)$ is defined by

$$w(p)=\frac{\pi}{\Gamma(p)\sin\left[\frac{(p-1)\pi}{2}\right]} \tag{21}$$

and $\Gamma(p)$ is the Gamma function. Approximating the sum in Eq. (17) by an integral and using expression (21) we find the critical temperature

$$\frac{T_c}{J}=\frac{(2-p)\pi^p}{2\Gamma(p)\sin\left[\frac{(p-1)\pi}{2}\right]}. \tag{22}$$

We see that the Green's function method predicts the existence of an ordering transition when $1<p<2$. Using the low-k expression in two dimensions given in Ref. 13, we can show that the Green's function method correctly predicts the condition $2<p<4$ for the existence of phase transition in two dimensions.

Using the standard asymptotic behavior of the Gamma function near $p=1$,[17] i.e., for $p\approx 1+\alpha$, where $|\alpha|\leqslant 3\times 10^{-7}$, we have

$$\Gamma(p)=p!\approx 1+\alpha p. \tag{23}$$

Therefore the critical temperature can be estimated as

$$\frac{T_c}{J}=\frac{1}{\alpha(1-b\alpha)}, \tag{24}$$

where $b=0.57719$.

To conclude, it would be interesting to compare the critical temperature given by Eq. (22) with other theoretical values given in the literature. For $p=\frac{3}{2}$ the numerical value of the critical temperature found from Eq. (22) is $T_c=2.23J$. By performing the sum given by Eq. (17) numerically, we obtain this same value of the critical temperature.

Using the simulation of the one-dimensional plane rotator, Romanos[18] found that $T_c=(2.16+0.01)J$. For the one-dimensional spherical model of Joyce,[19] we have $T_c=2.5128785J$. In conclusion, we have calculated the critical temperature in one-dimensional spin $-\frac{1}{2}$ Heisenberg ferro-

magnetic chain, with long-range interactions using the Green's function technique. For finite temperature, in contrast with the well-known Mermin-Wagner Theorem which cannot achieve long-range order (LRO) in pure one-dimensional Heisenberg systems because of the effect of quantum and thermal fluctuations.[20] When there is some interaction between spins decaying as r^{-p}, these fluctuations may be depressed to a certain extent and the system may realize LRO. The transition temperature can then be estimated as a function of p.

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