Green's function method applied to the crossover of the one-dimensional quantum anisotropic Heisenberg ferromagnet

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The spin-S quantum Heisenberg ferromagnet with anisotropic spin exchange interactions in one dimension is investigated by means of the Green's function method. The magnetic properties of this model are found to be dependent of the anisotropy. It is shown that the crossover of the anisotropic system to Heisenberg isotropic behavior happens at high temperatures $T \gg T_1$, and to an XY kind of behavior at some low temperatures $T \leqslant T_2$. For $S=1/2$ ferromagnetic chain system $(C_6H_{11}NH_3)CuBr_3$, our prediction of the crossover temperature T_2 and inverse correlation lengths are in agreement with the experiment results and numerical calculations.

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I. INTRODUCTION

In recent years one-dimensional magnetic systems have attracted a great deal of theoretical and experimental interest.[1] Several theoretical techniques have been employed to understand the magnetic properties of these systems. High-temperature series expansions,[2] spin-wave theory,[3,4] Monte Carlo method,[5] renormalization group analysis,[6,7] conformal field theory,[8] and the Green's function approach[9,10] are some of the methods used in these studies.

The two-time Green's function method used in Refs. 9 and 10 is known as the standard method in the study of magnetic systems.[11] In this method one obtains a nonlinear differential equation in which the higher-order Green's functions are coupled with the lower-order ones. Each of the higher-order Green's functions is again written down in the form of a nonlinear equation and so on. To obtain tractable solutions, decoupling procedures have been invoked to terminate the hierarchy of Green's functions generated by the equations of motion. Many results for the thermodynamic properties in three-dimensions have been obtained[12–17] in a frame of the simplest decoupling, i.e., the Tyablikov decoupling.[18] The decoupling provides a simple enough way for giving results in good agreement with other approaches and experiments in a wide range of temperatures and magnetic fields.

The Tyablikov decoupling is still valid even in fewer than three dimensions. Yablonskiy[9] used it to study the equilibrium properties of one- and two-dimensional isotropic quantum Heisenberg models, giving good qualitative agreement with the modified spin-wave theory[4] and the Schwinger bosonic and fermionic representation.[19] Hamedoun *et al.*[10] applied this method to quantum Heisenberg models with long-range ferromagnetic interaction, and found that there exists a phase transition at a finite temperature in contrast with the well-known Mermin-Wagner theorem.[20]

In this paper, we apply the Tyablikov decoupling, and provide a simple way to obtain the static properties of the spin-S quantum Heisenberg ferromagnet with anisotropic spin-exchange interactions in one dimension. The zero-temperature properties of this system are known.[21] Our motivation to study this problem is less of an analytical study on the crossover of one-dimensional finite-temperature properties of the anisotropic system than it is to study the isotropic or the XY properties. Most numerical and experimental studies are confined to the weak anisotropy for $S=1/2$. The crossover to an XY kind of behavior was observed experimentally at temperature $T \approx 4$ K for the $S=1/2$ ferromagnetic chain system $(C_6H_{11}NH_3)CuBr_3$ (CHAB).[22] The agreement with experiment was found from some numerical analysis[23] and the transfer-matrix calculations.[24] Campana *et al.*[7] estimated the crossover temperature $T \leqslant 10$ K in the framework of the real-space renormalization-group approach. However, those works failed to explain how the crossover behavior is dependent upon the exchange interaction J and the anisotropic parameter b. In this work, we show that anisotropy can have a rather drastic effect on the correlation functions and susceptibilities for any S. It is found that the crossover of the anisotropic system to Heisenberg isotropic behavior happens at high temperatures $T \gg T_1 = \frac{4}{3}S(S+1)J(1-b^2)^{1/2}$, and to an XY kind of behavior at some low temperatures below $T_2 \leqslant 2T_1/[1+b/(b-1+\sqrt{1-b^2})]$.

In Sec. II, using the formalism of the Green's function, we present the basic self-consistent equations for the correlation functions. In Sec. III the magnetic properties of this model are found to be dependent of anisotropy. The crossover with respect to anisotropy is explored. Section IV contains the discussions and conclusions.

II. MODEL

In this paper we will apply Green's function method with the Tyablikov decoupling to the spin-S quantum Heisenberg ferromagnet with anisotropic spin-exchange interactions. Its Hamiltonian is given by

$$H = -J\sum_{\langle i,j\rangle}[S_i^z S_j^z + S_i^x S_j^x + bS_i^y S_j^y] - h\sum_i S_i^z, \tag{1}$$

where the summation is taken over all nearest-neighbor pairs on a one-dimensional lattice. S_i^x, S_i^y and S_i^z represent the three components of the spin-S operator for a spin at site **i**. J is the exchange interaction, b denotes the anisotropic parameters with $0<b<1$. The magnetic field h is applied along the z axis. Here we have chosen the xz plane as the easy plane, and the y direction as the hard axis of magnetization. The above

Hamiltonian stands for isotropic ferromgnets for $b=1$, the XY model for $b=0$. For $S=1/2$ the model (1) can describe the compounds CHAB.

It is convenient to introduce the spin raising and lowering operators $S_i^{\pm}=S_i^x\pm iS_i^y$, which satisfies the commutation relations $[S_i^+,S_j^-]=2S_i^z\delta_{ij}$ and $[S_i^{\pm},S_j^z]=\mp S_i^{\pm}\delta_{ij}$. Then the above Hamiltonian can be rewritten as

$$H=-J\sum_{\langle i,j\rangle}\left[S_i^zS_j^z+\frac{1+b}{4}(S_i^+S_j^-+S_i^-S_j^+)+\frac{1-b}{4}(S_i^+S_j^++S_i^-S_j^-)\right]-h\sum_i S_i^z. \tag{2}$$

In order to calculate the magnetic properties of this model, we introduce two retarded Green's functions $\langle\langle S_i^{\pm}(t);e^{aS_j^z}S_j^-\rangle\rangle$, as

$$\langle\langle S_i^{\pm}(t);e^{aS_j^z}S_j^-(t')\rangle\rangle=-\imath\Theta(t-t')\langle[S_i^+(t),e^{aS_j^z}S_j^-(t')]\rangle. \tag{3}$$

Here $\langle A(t)\rangle\equiv\mathbf{Tr}[A(t)e^{-\beta H}]/\mathbf{Tr}[e^{-\beta H}]$, and $A(t)=e^{\imath Ht}Ae^{-\imath Ht}$, where β is the inverse of the temperature T. $\Theta(t)$ is the step function, and a is the Callen parameter.[12] The equations of motion for these two Green's functions follow in a straightforward fashion, which are given by

$$\begin{aligned}\imath\frac{d}{dt}\langle\langle S_i^+(t);e^{aS_j^z}S_j^-\rangle\rangle&=\delta(t)\delta_{ij}\theta(a)+h\langle\langle S_i^+(t);e^{aS_j^z}S_j^-\rangle\rangle\\&\quad+J\sum_\rho[2\langle\langle S_{i+\rho}^z(t)S_i^+(t);e^{aS_j^z}S_j^-\rangle\rangle\\&\quad-(1+b)\langle\langle S_i^zS_{i+\rho}^+(t);e^{aS_j^z}S_j^-\rangle\rangle\\&\quad-(1-b)\langle\langle S_i^zS_{i+\rho}^-(t);e^{aS_j^z}S_j^-\rangle\rangle],\end{aligned} \tag{4}$$

$$\begin{aligned}\imath\frac{d}{dt}\langle\langle S_i^-(t);e^{aS_j^z}S_j^-\rangle\rangle&=-h\langle\langle S_i^-(t);e^{aS_j^z}S_j^-\rangle\rangle\\&\quad-J\sum_\rho[2\langle\langle S_{i+\rho}^z(t)S_i^-(t);e^{aS_j^z}S_j^-\rangle\rangle\\&\quad-(1+b)\langle\langle S_i^zS_{i+\rho}^-(t);e^{aS_j^z}S_j^-\rangle\rangle-(1-b)\\&\quad\times\langle\langle S_i^zS_{i+\rho}^+(t);e^{aS_j^z}S_j^-\rangle\rangle].\end{aligned} \tag{5}$$

Here $\theta(a)=\langle[S^+;e^{aS^z}S^-]\rangle$ with $\theta(a=0)=2\langle S^z\rangle$. According to the Tyablikov decoupling,[18] we approximate the higher-order Green's functions on the right-hand sides of the above equations as

$$\langle\langle S_l^z(t)S_i^{\pm}(t);e^{aS_j^z}S_j^-\rangle\rangle=m\langle\langle S_i^{\pm}(t);e^{aS_j^z}S_j^-\rangle\rangle.$$

Here the value of magnetization $\langle S_i^z\rangle$ is considered to be independent of its site i, and setting $\langle S_i^z\rangle=m$ for any site i.

After Fourier transforming these equations with respect to the space and time variables, we obtain a set of algebraic equations that are readily solved for the transformed Green's functions $g_k(\omega)$ and $f_k(\omega)$ of $\langle\langle S_i^+(t);e^{aS_j^z}S_j^-\rangle\rangle$, and $\langle\langle S_i^-(t);e^{aS_j^z}S_j^-\rangle\rangle$, respectively. The solutions that are found can be written

$$g_k(\omega)=\theta(a)(\omega+E_1+h)/(\omega^2-\omega_k^2), \tag{6}$$

$$f_k(\omega)=\theta(a)E_2/(\omega^2-\omega_k^2), \tag{7}$$

where

$$\omega_k=[(h+E_1)^2-E_2^2]^{1/2}, \tag{8}$$

$$E_1=2mJ[2-(1+b)\cos k], \tag{9}$$

$$E_2=2mJ(1-b)\cos k. \tag{10}$$

From the spectral theorem and the solutions of the Green's functions (6) and (7), we find the correlation functions

$$\langle e^{aS_j^z}S_j^-S_i^{\pm}(t)\rangle=\frac{1}{N}\sum_k e^{\imath\mathbf{k}\cdot(\mathbf{i}-\mathbf{j})}G^{-\pm}(k,t). \tag{11}$$

Here $G^{-+}(k,t)$ and $G^{--}(k,t)$ are the correlation functions in the momentum space. They are

$$G^{-+}(k,t)=\frac{\theta(a)}{2}\left(\frac{e^{-\imath\omega_kt}}{\omega_k}\frac{\omega_k+E_1+h}{e^{\beta\omega_k}-1}+\frac{e^{\imath\omega_kt}}{\omega_k}\frac{\omega_k-E_1-h}{e^{-\beta\omega_k}-1}\right), \tag{12}$$

$$G^{--}(k,t)=\frac{\theta(a)}{2}\frac{E_2}{\omega_k}\left(\frac{e^{-\imath\omega_kt}}{e^{\beta\omega_k}-1}-\frac{e^{\imath\omega_kt}}{e^{-\beta\omega_k}-1}\right). \tag{13}$$

Similarly, we may also calculate the correlation functions $\langle e^{aS_j^z}S_j^{\alpha}S_i^{\alpha}(t)\rangle$, with $\alpha=x,y$. Setting $t=0$ and for $a=0$, we find

$$\langle S_j^xS_i^x\rangle=\frac{1}{N}\sum_k e^{\imath\mathbf{k}\cdot(\mathbf{i}-\mathbf{j})}m\frac{h+E_1+E_2}{2\omega_k}\coth\frac{\beta\omega_k}{2}, \tag{14}$$

$$\langle S_j^yS_i^y\rangle=\frac{1}{N}\sum_k e^{\imath\mathbf{k}\cdot(\mathbf{i}-\mathbf{j})}m\frac{h+E_1-E_2}{2\omega_k}\coth\frac{\beta\omega_k}{2}. \tag{15}$$

When $i=j$ and $t=0$ in Eq. (11) for $a=0$, and using the relation

$$\langle S_i^-S_i^+\rangle=S(S+1)-\langle S_i^z\rangle-\langle(S_i^z)^2\rangle,$$

we have the magnetization $m=\langle S_i^z\rangle$ which is obtained from a solution of the equations

$$m=\frac{(S-\phi)(1+\phi)^{2S+1}+(S+1+\phi)\phi^{2S+1}}{(1+\phi)^{2S+1}-\phi^{2S+1}}, \tag{16}$$

$$2\phi+1=\frac{1}{N}\sum_k\frac{E_1+h}{\omega_k}\coth\frac{\beta\omega_k}{2}. \tag{17}$$

III. MAGNETIC PROPERTIES

In this section, we use our solutions of the Green's functions to derive formulas for the magnetic properties as a function of temperature and anisotropy for the case S.

In the following, we will firstly calculate the temperature and anisotropy dependence of the uniform-field susceptibility χ and the equal-time correlation functions $\langle S_0^{\alpha}S_n^{\alpha}\rangle$, $\alpha=x,y$, in the paramagnetic phase. The susceptibility when the applied field is small is defined by $\chi = m/h$. From Eqs. (14)–(17) we obtain for the equations which determine the susceptibility and the equal-time correlation functions at temperature $T>0$. The results are

$$\frac{8}{3}S(S+1)\beta J = \{[1+1/(4\chi J)]^2-1\}^{-1/2} + \{[1+1/(4\chi J)]^2-b^2\}^{-1/2}, \qquad (18)$$

$$\langle S_0^x S_n^x\rangle = (4\beta J \sinh \kappa_x)^{-1} e^{-\kappa_x n}, \qquad (19)$$

$$\langle S_0^y S_n^y\rangle = (4b\beta J \sinh \kappa_y)^{-1} e^{-\kappa_y n}. \qquad (20)$$

Here κ^α is the so-called inverse correlation length for the spin components S^α, $\alpha = x, y$, which are given by

$$1+\frac{1}{4\chi J} = \cosh \kappa_x = b \cosh \kappa_y. \qquad (21)$$

For any $T>0$ and $b<1$, $\langle S_0^y S_n^y\rangle < \langle S_0^x S_n^x\rangle$ and $\kappa_x<\kappa_y$. This may be explained by the fact that the anisotropy has an tendency to destroy the growth of the correlation along the hard axis. It is shown that as the temperature and anisotropy vary, the behavior of the anisotropic system changes smoothly from an XY type (if $b=0$) to an isotropic type (if $b=1$). Equation (18) suggests that no transitions at finite temperature exist in one dimension, which agrees with the Mermin-Wagner theorem,[20] and is a fundamental difference from the corresponding three-dimensional case.[14]

For $[(1+1/4\chi J)^2-1]/(1-b^2) \gg 1$, i.e.,

$$T \gg T_1 = \frac{4}{3}S(S+1)J\sqrt{1-b^2}, \qquad (22)$$

the behavior of the system crosses over to the Heisenberg isotropic behavior, with very small corrections due to the anisotropy. In this case, Eqs. (18) and (21) can be calculated to be

$$\chi = \frac{1}{4J}[\sqrt{1+(1-T_1^2\beta^2/4)^2/(\tilde{\beta}J)^2}-1]^{-1}, \qquad (23)$$

$$\kappa_x = -\ln[\sqrt{1+(1+T_1^2\beta^2/4)^2/(\tilde{\beta}J)^2}-(1-T_1^2\beta^2/4)/(\tilde{\beta}J)]. \qquad (24)$$

$$\kappa_y = -\ln[\sqrt{1+(1-T_1^2\beta^2/4)^2/(\tilde{\beta}J)^2}-(1+T_1^2\beta^2/4)/(\tilde{\beta}J)]. \qquad (25)$$

To the zero order of b, they agree with Ref. 9. Here $\tilde{\beta} = 4S(S+1)\beta/3$. To the nontrivial order of b, one will find the corrections to the behavior due to the anisotropy in the following two limit cases. For $T_1 \ll T \ll \frac{4}{3}S(S+1)J$,

$$\chi = \frac{1}{2}\tilde{\beta}^2 J(1+T_1^2\beta^2/2), \qquad (26)$$

$$\langle S_0^x S_n^x\rangle = \frac{1}{3}S(S+1)(1+T_1^2\beta^2/4)e^{-\kappa_x n}, \qquad (27)$$

$$\langle S_0^y S_n^y\rangle = \frac{1}{3}S(S+1)(1-T_1^2\beta^2/4)e^{-\kappa_y n}, \qquad (28)$$

where $\kappa_x = (\tilde{\beta}J)^{-1}$ and $\kappa_y = (1-\tilde{\beta}J\ln b)/(\tilde{\beta}J)$. If $b=1$, those agree with the isotropic result,[9] and qualitatively coincide with the modified spin-wave theory[4] and the Schwinger bosonic and fermionic representation.[19]

In the case of $T \gg \frac{4}{3}S(S+1)J$, the susceptibility is approximately

$$\chi = \tilde{\beta}[1+\tilde{\beta}J+\tilde{\beta}^2J^2(3-b^2)/4]/4. \qquad (29)$$

This indicates that the anisotropy is devoted to the susceptibility only in order of T^{-3}. This is similar to a three-dimensional situation.[17] However, the anisotropic effect is more pronounced in one dimension. In this case the correlations have same expressions as Eqs. (27) and (28), but with different inverse lengths $\kappa_x = \ln[2/(\tilde{\beta}J)]$ and $\kappa_y = \ln[2/(b\tilde{\beta}J)]$.

Let us consider the opposite region $T<T_1$. For $[(1+1/4\chi J)^2-1]/(1-b^2) \ll 1$, i.e., $T \ll T_1$, the behavior of the system crosses over to the XY behavior,[25] with the corrections due to the anisotropy. The results are

$$\chi = \frac{1}{4J}[\sqrt{1+(1-b^2)(2T_1/T-1)^{-2}}-1]^{-1}, \qquad (30)$$

$$\langle S_0^x S_n^x\rangle = \frac{1}{3}S(S+1)(2-T/T_1)e^{-\kappa_x n}, \qquad (31)$$

$$\langle S_0^y S_n^y\rangle = \frac{T}{3T_1}S(S+1)e^{-\kappa_y n}, \qquad (32)$$

$$\kappa_x = -\ln[\sqrt{1+(1-b^2)(2T_1/T-1)^{-2}}-\sqrt{1-b^2}(2T_1/T-1)^{-1}], \qquad (33)$$

$$\kappa_y = -\ln\{[\sqrt{1+(1-b^2)(2T_1/T-1)^{-2}} - \sqrt{1-b^2}\sqrt{1+(2T_1/T-1)^{-2}}]/b\}. \qquad (34)$$

It is noted that κ_y is independent of the temperature T in the nontrivial order of b. As $T\to 0$, $\kappa_x = (2\tilde{\beta}J)^{-1}$ diverges, as in the XY case. In order to estimate the crossover temperature T_2, we may choose $[(1+1/4\chi J)^2-1]/(1-b^2) = c$ as a variable parameter instead of T. In our case, c takes the value of $(2T_1/T-1)^{-2}$ which yields the condition $c \ll 1$. To the nontrivial order of $\sqrt{c}$ in the argument, κ_y is found to be $-\ln[(1-\sqrt{1-b^2})/b]$, and the upper limit of κ_x is approximately to be $-\ln(1-\sqrt{c})$. Since $\kappa_x<\kappa_y$ in the XY case, we obtain $c<(b-1+\sqrt{1-b^2})^2/b^2$. Then the crossover of the anisotropic system towards the XY kind of behavior is estimated at low temperatures T below

$$T_2 \leq 2T_1/[1+b/(b-1+\sqrt{1-b^2})]. \qquad (35)$$

IV. CONCLUSIONS AND DISCUSSIONS

In this paper we studied the magnetic properties of the spin-S one-dimensional quantum anisotropic Heisenberg ferromagnet by means of the Green's function method. The magnetic properties of this model are found to be dependent on the anisotropy. Since the magnetic anisotropy tends to suppress part of the fluctuation along the the hard (y) axis, for any $T>0$ and $b<1$, the correlation $\langle S_0^y S_n^y \rangle$ is always smaller than $\langle S_0^x S_n^x \rangle$. As the temperature decreases and enters in the low-temperature region of $T<T_2$, the anisotropy strongly destroys the thermal fluctuations along the hard axis so that the correlation $\langle S_0^y S_n^y \rangle \ll \langle S_0^x S_n^x \rangle$. This means that the anisotropic system exhibits an XY kind of behavior. However, as the temperature gets larger, the fluctuations due to the thermal motion of the spins are more intensive. At very high temperature $T \gg T_1$, all spin components have to tendency to display the same number of fluctuations, which leads us to conclude that the system behaves as it does in the isotropic case. Although the anisotropic effect is very weak at very high temperatures, the anisotropy gives rise to very small corrections to the isotropic behavior. As seen in Eqs. (23)–(29), it is shown that the anisotropy plays different roles in the xx and yy correlations. As compared with the isotropic case, the anisotropy destroys the growth of the correlation along the hard axis, but helps the growth of the correlation along the easy axes.

Due to the anisotropy, there exist two different kinds of inverse correlation lengths κ_x and κ_y for $b<1$. And $\kappa_x < \kappa_y$ is hold for $T>0$. As the parameter b increases (i.e., the anisotropy gets weak), the difference between κ_x and κ_y decreases. κ_x is less dependent on the anisotropy than κ_y. Above T_1, Eq. (21) describes the isotropic correlation length [as seen in Eqs. (24) and (25) for $b=1$] fairly well. In Eq. (32), the out-of-plane (yy) correlation vanishes for $T \to 0$, which results from the limiting of spin fluctuation perpendicular to the easy xz plane. In the low-temperature region $T<T_2$, quantum mechanics can effectively confine spins in the easy plane, as in the XY model.[26,27] Therefore the low-temperature properties of the system are mainly dominated by the spin components within the easy plane.

Because CHAB is a $S=1/2$ nearly isotropic quantum system which can be described by model (1), it is interesting to compare our results with those of the experimental and theoretical studies. In the case of $S=1/2$, taking $b=0.95$ and $J=55$ K,[22] we estimate the characteristic temperature $T_1=17.17$ K, the crossover temperature $T_2 \leq 7.43$ K, and the small parameter $c<0.0762$. The value of T_2 is in agreement with $T_2 \approx 4$ K for CHAB by neutron scattering experiment,[22] 4.5 K by numerical calculations,[23] and 3 K by transfer-matrix calculations.[24] And it is comparable to $T_2 \leq 10$ K by renormalization-group approach.[7] For $T<T_1$, the inverse correlation length κ_y takes the value of 0.323, which agrees with the range from 0.3 to 0.4 (Refs. 24 and 22) and is smaller than 0.44 (Ref. 23) Our κ_x is consistent with Ref. 23 in each asymptotic region. If one wants to get more properties (such as specific heat) in agreement with experiment and numerical calculations, he may choose the Kondo-Yamaji decoupling technique[28] (which is at a stage one step further than the Tyablikov decoupling) to deal with the Green's functions. This will be left for the coming work.

In this work, we show that anisotropy can have a rather drastic effect on the correlation functions and susceptibilities for any S. The magnetic properties of this model are found to be dependent on the anisotropy. It is found that the crossover of the anisotropic system to Heisenberg isotropic behavior happens at high temperatures $T \gg T_1$, and to an XY kind of behavior at some low temperature $T \leq T_2$.

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