Schwinger-boson mean-field theory of the Heisenberg ferrimagnetic spin chain

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(Received 16 November 1998)

The Schwinger-boson mean-field theory is applied to the quantum ferrimagnetic Heisenberg chain. There is a ferrimagnetic long-range order in the ground state. We observe two branches of the low-lying excitation and calculate the spin reduction, the gap of the antiferromagnetic branch, and the spin fluctuation at $T=0$ K. These results agree with the established numerical results quite well. At finite temperatures, the long-range order is destroyed because of the disappearance of the Bose condensation. The thermodynamic observables, such as the free energy, magnetic susceptibility, specific heat, and the spin correlation at $T>0$ K, are calculated. The $T\chi_{uni}$ has a minimum at intermediate temperatures and the spin-correlation length behaves as T^{-1} at low temperatures. These qualitatively agree with the numerical results and the difference is small at low temperatures. [S0163-1829(99)07225-2]

I. INTRODUCTION

A variety of exotic physical phenomena in the low-dimensional magnetic systems have been attracting much interest in recent years. In these systems, the physical pictures obtained from the classical approach are often greatly modified or even in contradiction with the result of the strong quantum fluctuation and topological effect. Haldane[1] conjectured that the one-dimensional integer-spin chain with the nearest-neighbor coupling has an energy gap in the spin excitation spectrum and the spin correlation decays exponentially with distance, whereas that of the half-odd-integer spin chain is gapless and the spin correlation decays algebraically with distance.

It is very interesting to discuss the physical phenomena for the spin chain mixed by different kinds of spins. Recently, the one-dimensional Heisenberg ferrimagnetic spin chain, which is made of two kinds of spins, $S^A=1/2$ and $S^B=1$, has been considered.[2–8] This one-dimensional chain can be described by the Hamiltonian

$$H=\sum_{i=1,\eta}^{N}\vec{S}_i^A\cdot\vec{S}_{i+\eta}^B, \tag{1}$$

where the antiferromagnetic coupling energy J is set to equal 1. N is the number of unit cells, and η is the index of the nearest neighbors. Brehmer *et al.*[2] showed that the absolute ground state of this model has a ferrimagnetic long-range order and obtained the low-lying excitation, by using the spin-wave theory (SWT) and the quantum Monte Carlo method (QMC), which is confirmed by Kolezhuk *et al.*[3] with the matrix product approach. It is also consistent with Tian's[8] rigorous theorem that the absolute ground state for the one-dimensional antiferromagnetic Heisenberg model with unequal spins has both antiferromagnetic and ferromagnetic long-range orders. Furthermore, Yamamoto *et al.*[6] used the modified spin-wave theory (MSWT), the density-matrix renormalization-group method (DMRG) and QMC to calculate the thermodynamic observables.

In this paper we study the ferrimagnetic spin chain by means of the Schwinger-boson mean-field theory (SBMFT). The theory has been applied successfully to the integer Heisenberg chain,[9] presumably due to the neglect of topological excitations in the SBMFT. It can also be extended to the case of the magnetic order range[11] by identifying the magnetic order with the Bose condensation of the Schwinger bosons. In the Heisenberg ferrimagnetic spin chain, we find that the SMBFT theory is suitable to describe both the ground state with the ferrimagnetic long-range order and the thermodynamic properties at finite temperatures. The mean-field theory gives rise to the leading term in a systematic $1/N$ expansion[9] and the effects of fluctuation beyond the mean-field theory can also be discussed, as we will mention later.

In our SBMFT approach, the ground state has a long-range ferrimagnetic order arising from the condensation of the Schwinger bosons at $T=0$ K. There are two different kinds of excitation: One is gapless and ferromagnetic and the other is gapful and antiferromagnetic, which has been pointed out by Brehmer *et al.*[2] The spin reduction, the gap of the antiferromagnetic branch, and the spin correlation at $T=0$ K are calculated and the results are in good agreement with those of the QMC and DMRG.[2,6] When $T>0$ K, the two branches of excitation are both gapful, so that the Bose condensation disappears and there is no real long-range order. This is just what the Wigner-Mermin theorem tells us for one dimension. The gap of the ferromagnetic branch is proportional to T^2 and the spin-correlation length is divergent as $1/T$. The thermodynamic observables, such as the free energy, the magnetic susceptibility, and the specific heat, are calculated. They agree with the numerical results[2,6] qualitatively and the difference is small at low temperatures.

This paper is organized as follows: In the second section we construct the mean-field theory of the ferrimagnetic chain. In the third section we give the ground-state properties. In the fourth section we study the thermodynamic properties. Conclusions are made and advantages and limitations compared with other approaches are discussed in the final section.

II. SCHWINGER-BOSON MEAN-FIELD THEORY OF THE FERRIMAGNTIC HEISENBERG SPIN CHAIN

The spin operator $\vec{S}_i^A$ can be represented by the Schwinger bosons $a_{i,\uparrow}, a_{i,\downarrow}$,

$$S_{i,+}^A = a_{i,\uparrow}^\dagger a_{i,\downarrow} \quad S_{i,-}^A = a_{i,\downarrow}^\dagger a_{i,\uparrow},$$

$$S_{i,z}^A = \frac{1}{2}(a_{i,\uparrow}^\dagger a_{i,\uparrow} - a_{i,\downarrow}^\dagger a_{i,\downarrow}), \tag{2}$$

with $S_i^A = \frac{1}{2}(a_{i,\uparrow}^\dagger a_{i,\uparrow} + a_{i,\downarrow}^\dagger a_{i,\downarrow})$ on each site of kind A, and $\vec{S}_j^B$ can be represented in a similar way.

The Hamiltonian (1) is rewritten in this representation,

$$H = -\frac{1}{2}\sum_{i=1,\eta}^{N}(a_{i,\uparrow}^\dagger b_{i+\eta,\downarrow}^\dagger - a_{i,\downarrow}^\dagger b_{i+\eta,\uparrow}^\dagger) \times (a_{i,\uparrow} b_{i+\eta,\downarrow} - a_{i,\downarrow} b_{i+\eta,\uparrow}) + \sum_{i,\eta} S_i^A S_{i+\eta}^B$$
$$= -2\sum_{i=1,\eta}^{N} D_{i,i+\eta}^\dagger D_{i,i+\eta} + \sum_{i,\eta} S_i^A S_{i+\eta}^B, \tag{3a}$$

$$D_{i,i+\eta} = \frac{1}{2}(a_{i,\uparrow} b_{i+\eta,\downarrow} - a_{i,\downarrow} b_{i+\eta,\uparrow}). \tag{3b}$$

Considering the constraint $\Sigma_\sigma a_{i,\sigma}^\dagger a_{i,\sigma} = 2S^A$ or $\Sigma_\sigma b_{j,\sigma}^\dagger b_{j,\sigma} = 2S^B$ on each site, we may introduce two kinds of Lagrangian multipliers λ_i^A and λ_j^B to impose the constraint. At the mean-field level, we can take the average value of the bond operator $\langle D_{i,i+\eta}\rangle = D$ to be uniform and static. And so are $\langle \lambda_i^A \rangle = \lambda^A$ and $\langle \lambda_j^B \rangle = \lambda^B$.

The mean-field Hamiltonian reads

$$H_{MF} = -\sum_{i=1,\eta}^{N}\{D^*(a_{i,\uparrow} b_{i+\eta,\downarrow} - a_{i,\downarrow} b_{i+\eta,\uparrow}) + (a_{i,\uparrow}^\dagger b_{i+\eta,\downarrow}^\dagger - a_{i,\downarrow}^\dagger b_{i+\eta,\uparrow}^\dagger)D\} \tag{4a}$$

$$+\lambda^A \sum_{i=1}^{N}(a_{i,\sigma}^\dagger a_{i,\sigma} - 2S^A) + \lambda^B \sum_{j=1}^{N}(b_{j,\sigma}^\dagger b_{j,\sigma} - 2S^B) + 2zND^*D + zNS^AS^B, \tag{4b}$$

in momentum space, which is transformed into

$$H_{MF} = \sum_{k,\sigma}\{\lambda^A a_{k,\sigma}^\dagger a_{k,\sigma} + \lambda^B b_{k,\sigma}^\dagger b_{k,\sigma}\} - \sum_{k,\sigma}\{D^* z\gamma_k^*(a_{k,\uparrow} b_{-k,\downarrow} - a_{k,\downarrow} b_{-k,\uparrow}) + Dz\gamma_k(a_{k,\uparrow}^\dagger b_{-k,\downarrow}^\dagger - a_{k,\downarrow}^\dagger b_{-k,\uparrow}^\dagger)\} + 2zND^*D - 2N(S^A\lambda^A + S^B\lambda^B) + zNS^AS^B. \tag{4c}$$

Here z is the number of the nearest-neighbor sites and equals 2 in the one-dimensional chain, and $\gamma_k = (1/z)\Sigma_\eta e^{ik\eta} = \cos k$. The sum of k is restricted in the reduced first Brillouin zone, which extends from $-\pi/2$ to $\pi/2$.

Using the Bogoliubov transformation

$$\begin{pmatrix} a_{k,\uparrow} \\ b_{-k,\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} \cosh\theta_k & \sinh\theta_k \\ \sinh\theta_k & \cosh\theta_k \end{pmatrix}\begin{pmatrix} \alpha_{k,\uparrow} \\ \beta_{-k,\downarrow}^\dagger \end{pmatrix} \quad \begin{pmatrix} b_{k,\uparrow} \\ a_{-k,\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} \cosh\theta_k & -\sinh\theta_k \\ -\sinh\theta_k & \cosh\theta_k \end{pmatrix}\begin{pmatrix} \beta_{k,\uparrow} \\ \alpha_{-k,\downarrow}^\dagger \end{pmatrix}, \tag{5}$$

with θ given by

$$\tanh 2\theta = \frac{|zD\gamma_k|}{(\lambda^A + \lambda^B)/2}, \tag{6a}$$

we obtain the energy spectrum

$$E_{k,\sigma}^\alpha = \frac{\lambda^A - \lambda^B}{2} + \sqrt{\left(\frac{\lambda^A + \lambda^B}{2}\right)^2 - |zD\gamma_k|^2}, \tag{6b}$$

$$E_{k,\sigma}^\beta = -\frac{\lambda^A - \lambda^B}{2} + \sqrt{\left(\frac{\lambda^A + \lambda^B}{2}\right)^2 - |zD\gamma_k|^2}. \tag{6c}$$

The Hamiltonian is diagonalized and it is easy to write down the free energy,

$$H_{MF} = \sum_{k,\sigma}\{E_k^\alpha(\alpha_{k,\sigma}^\dagger \alpha_{k,\sigma} + 1/2) + E_k^\beta(\beta_{k,\sigma}^\dagger \beta_{k,\sigma} + 1/2)\} + 2zND^*D - 2N(S^A + 1/2)\lambda^A - 2N(S^B + 1/2)\lambda^B + zNS^AS^B \tag{7a}$$

$$\frac{F^{MF}}{2N} = \frac{2}{\beta}\int_{-\pi/2}^{\pi/2}\frac{dk}{2\pi}\left\{\ln\left[2\sinh\left(\frac{\beta}{2}E_k^\alpha\right)\right] + \ln\left[2\sinh\left(\frac{\beta}{2}E_k^\beta\right)\right]\right\} + zD^*D - (S^A + 1/2)\lambda^A - (S^B + 1/2)\lambda^B + \frac{z}{2}S^AS^B. \tag{7b}$$

The mean-field self-consistent equations can be obtained by minimizing the free energy, i.e., $\delta F/\delta\lambda^A = 0$, $\delta F/\delta\lambda^B = 0$, and $\delta F/\delta D^* = 0$. After a simple algebra, the equations are rearranged as

$$S^B - S^A = \int_{-\pi/2}^{\pi/2}\frac{dk}{2\pi}\left\{\coth\frac{\beta}{2}E_k^\beta - \coth\frac{\beta}{2}E_k^\alpha\right\}, \tag{8a}$$

$$S^B+S^A+1=\int_{-\pi/2}^{\pi/2}\frac{dk}{2\pi}\frac{(\lambda^A+\lambda^B)/2}{\sqrt{\left(\frac{\lambda^A+\lambda^B}{2}\right)^2-|zD\gamma_k|^2}}\times\left\{\coth\frac{\beta}{2}E_k^{\beta}+\coth\frac{\beta}{2}E_k^{\alpha}\right\}, \tag{8b}$$

$$\frac{2}{z}=\int_{-\pi/2}^{\pi/2}\frac{dk}{2\pi}\frac{|\gamma_k|^2}{\sqrt{\left(\frac{\lambda^A+\lambda^B}{2}\right)^2-|zD\gamma_k|^2}}\times\left\{\coth\frac{\beta}{2}E_k^{\beta}+\coth\frac{\beta}{2}E_k^{\alpha}\right\}. \tag{8c}$$

Rescale the parameters $(\lambda^A,\lambda^B,D,\beta)\to(\Lambda_1,\Lambda_2,\eta,\kappa)$ (Ref. 8):

$$\frac{\lambda^A+\lambda^B}{2}=\frac{1}{2}z\Lambda_1,\quad D=\frac{1}{2}\Lambda_1\eta,$$
$$\frac{\lambda^A-\lambda^B}{2}=\frac{1}{2}z\Lambda_2,\quad \beta=\frac{4\kappa}{z}. \tag{9}$$

Then the angle of the Bogoliubov transformation is expressed in a compact form

$$\cosh 2\theta_k=\frac{1}{\sqrt{1-\eta^2\gamma_k^2}},\quad \sinh 2\theta_k=\frac{|\eta\gamma_k|}{\sqrt{1-\eta^2\gamma_k^2}}, \tag{10}$$

and the self-consistent equations read

$$S^B-S^A=\int_0^{\pi/2}\frac{dk}{\pi}\{\coth[\kappa(\Lambda_1\sqrt{1-\eta^2\gamma_k^2}-\Lambda_2)]-\coth[\kappa(\Lambda_1\sqrt{1-\eta^2\gamma_k^2}+\Lambda_2)]\}, \tag{11a}$$

$$S^B+S^A+1=\int_0^{\pi/2}\frac{dk}{\pi}\left\{\frac{\coth[\kappa(\Lambda_1\sqrt{1-\eta^2\gamma_k^2}-\Lambda_2)]+\coth[\kappa(\Lambda_1\sqrt{1-\eta^2\gamma_k^2}+\Lambda_2)]}{\sqrt{1-\eta^2\gamma_k^2}}\right\}, \tag{11b}$$

$$S^B+S^A+1-\Lambda_1\eta^2=\int_0^{\pi/2}\frac{dk}{\pi}\{\coth[\kappa(\Lambda_1\sqrt{1-\eta^2\gamma_k^2}-\Lambda_2)]+\coth[\kappa(\Lambda_1\sqrt{1-\eta^2\gamma_k^2}+\Lambda_2)]\}\sqrt{1-\eta^2\gamma_k^2}. \tag{11c}$$

III. PROPERTIES OF THE GROUND STATE

Notice that the Bogoliubov particles in the β branch have to condense at $T=0$ K as long as $S^A\neq S^B$, otherwise Eq. (11a) cannot be satisfied. The excitation energy E_β has its minimal value $E_\beta=0$ at $k=0$ while the α branch has a gap of $2\Lambda_2$ at $T=0$ K. Sarker *et al.*[11] showed that the long-range order is related to the condensation of the Schwinger bosons in both the ferromagnetic and antiferromagnetic Heisenberg models. We now arrive at the same conclusion for the ferrimagnetism model at one dimension. This can be contrasted to the antiferromagnetic case, where there is no long-range order even at $T=0$ K at one dimension.

Suppose that there is an infinitesimal external stagger magnetic field that is upward at the B site and downward at the A site. Then the $\beta_\uparrow$ branch has the lowest energy and the bosons condense at the state of $\beta_{\uparrow,k=0}$. Because of the bose condensation, the self-consistent equations at $T=0$ K are modified as follows:

$$S^B-S^A=\frac{1}{4N}\coth[\kappa(\Lambda_1\sqrt{1-\eta^2}-\Lambda_2)]|_{\kappa\to+\infty}, \tag{12a}$$

$$\Lambda_1\sqrt{1-\eta^2}=\Lambda_2, \tag{12b}$$

$$S^B+S^A+1=\frac{2}{\pi}K(\eta)+\frac{(S^B-S^A)}{\sqrt{1-\eta^2}}, \tag{12c}$$

$$S^B+S^A+1-\Lambda_1\eta^2=\frac{2}{\pi}E(\eta)+(S^B-S^A)\sqrt{1-\eta^2}. \tag{12d}$$

Here $E(\eta)$ and $K(\eta)$ are the first- and second-type complete elliptic integrals. The parameters have been determined numerically for the case in $S^A=1/2$ and $S^B=1$ with $\eta=0.8868$, $\Lambda_1=1.9238$, and $\Lambda_2=0.8890$.

The average value of the spin on the site B,

$$\langle S_Z^B\rangle=\frac{1}{2}\langle b_{j\uparrow}^\dagger b_{j\uparrow}-b_{j\downarrow}^\dagger b_{j\downarrow}\rangle=\frac{1}{2N}\sum_k\langle b_{k\uparrow}^\dagger b_{k\uparrow}-b_{k\downarrow}^\dagger b_{k\downarrow}\rangle,$$

can be calculated at $T=0$ K, by using the quasiparticle operator

$$\langle S_Z^B\rangle=\frac{1}{2N}\cosh^2\theta_k n_{\beta k\uparrow}|_{k=0,T\to 0\ \mathrm{K}}$$
$$=\frac{1}{2}\left(1+\frac{1}{\sqrt{1-\eta^2}}\right)(S^B-S^A)=0.791. \tag{13a}$$

Similarly, the average value of the spin on the site A is

$$\langle S_Z^A\rangle=-\frac{1}{2N}\sinh^2\theta_k n_{\beta k\uparrow}|_{k=0,T\to 0\ \mathrm{K}}$$
$$=\frac{1}{2}\left(1-\frac{1}{\sqrt{1-\eta^2}}\right)(S^B-S^A)=-0.291. \tag{13b}$$

The spin reduction $\tau = S^B - \langle S_z^B \rangle$ on the site B or $\tau = S^A + \langle S_z^A \rangle$ on the site A is given by

$$\tau^A = \tau^B = \frac{(S^B + S^A)}{2} - \frac{1}{\sqrt{1-\eta^2}} \frac{(S^B - S^A)}{2} = 0.209. \tag{13c}$$

From Eq. (11a), we can see that the number of the condensed bosons on the state $\beta_{\uparrow,k=0}$ is $2N(S^B - S^A)$, which is just the number of the Schwinger bosons on the site B subtracted by that on the site A. As long as $S^A \neq S^B$, there is a ferrimagnetic long-range order, which agrees with Tian's rigorous proof.[8] We quote several known results for the value of τ to show the satisfactiom of our calculation. The QMC (Ref. 2) gives $\tau = 0.207 \pm 0.002$ and $\tau = 0.221$ in the matrix product states approach.[3] The naive SWT overestimates the spin reduction and results in $\tau = 0.3$.[2]

The gap of the antiferromagnetic branch in our mean-field theory is $\Delta_{anti} = 2\Lambda_2 = 1.778$, which is very close to that in the exact diagonalization,[4] $\Delta_{anti} = 1.759$, and in the QMC,[2] $\Delta_{anti} = 1.767$. The naive SWT (Ref. 2) and the MSWT (Ref. 6) give the gap $\Delta_{anti} = 1$ and $\Delta_{anti} = 1.676$, respectively.

We calculate the ground-state energy of one unit cell, which yields the zero-temperature free energy per unit cell,

$$\begin{aligned}\frac{F_{MF}}{N} &= \int_{-\pi/2}^{\pi/2} \frac{dk}{2\pi} \{4\Lambda_1 \sqrt{1-\eta^2\gamma_k^2}\} + \frac{z}{2}\Lambda_1^2 \eta^2 \\ &\quad - 2\Lambda_1 (S^A + S^B + 1) - 2\Lambda_2 (S^A - S^B) + z S^A S^B \\ &= -1.904. \end{aligned} \tag{14}$$

This result is much lower than those of the QMC (Ref. 2) and the MSWT,[6] which are -1.437 and -1.454, respectively. In fact, this is an artificial result caused by the mean-field theory, in which we assume that the constraint and the bond operator are uniform and static. We have overcounted the degrees of freedom of the Schwinger bosons by a factor of 2, as argued by Arovas and Auerbach.[9,10] To count the degrees of freedom correctly, we have to divide the part of fluctuation per unit cell $F_{MF}/N + 2S^A S^B$ by 2, and add back the classic ground energy per cell $-2S^A S^B$. Then we have the modified result, -1.455. The $1/N$ expansion can give the above argument a strong basis.

The spin-correlation length ξ of the ground state is also of interest. Because of the appearance of the long-range order, the transverse and longitudinal fluctuations are anisotrope. In our SBMFT, the longitudinal correlation between the site A and the site B can be calculated as

$$\begin{aligned}&\langle S_{i,z}^A S_{j,z}^B \rangle - \langle S_{i,z}^A \rangle \langle S_{j,z}^B \rangle \\ &\quad = -\langle (S^A - a_{i,\uparrow}^\dagger a_{i,\uparrow})(S^B - b_{j,\downarrow}^\dagger b_{j,\downarrow}) \rangle + \langle (S^A - a_{i,\uparrow}^\dagger a_{i,\uparrow}) \rangle \\ &\qquad \times \langle (S^B - b_{j,\downarrow}^\dagger b_{j,\downarrow} \rangle \\ &\qquad = -\langle a_{i,\uparrow}^\dagger a_{i,\uparrow} b_{j,\downarrow}^\dagger b_{j,\downarrow} \rangle + \langle a_{i,\uparrow}^\dagger a_{i,\uparrow} \rangle \langle b_{j,\downarrow}^\dagger b_{j,\downarrow} \rangle \\ &\qquad = -|g(R_{ij})|^2, \end{aligned} \tag{15a}$$

$$g(R_{ij}) = \int_{-\pi/2}^{\pi/2} \frac{dk}{2\pi} \sinh 2\theta_k e^{-ikR_{ij}}. \tag{15b}$$

Similarly, the longitudinal fluctuations between A site and A site and between B site and B site can be given by

$$\langle S_{i,z}^A S_{j,z}^A \rangle - \langle S_{i,z}^A \rangle \langle S_{j,z}^A \rangle = |f(R_{ij})|^2, \tag{15c}$$

$$\langle S_{i,z}^B S_{j,z}^B \rangle - \langle S_{i,z}^B \rangle \langle S_{j,z}^B \rangle = |f(R_{ij})|^2, \tag{15d}$$

$$f(R_{ij}) = \int_{-\pi/2}^{\pi/2} \frac{dk}{2\pi} \cosh 2\theta_k e^{-ikR_{ij}}. \tag{15e}$$

From Eqs. (15b) and (15e) we get the correlation length $\xi = \eta/[8(1-\eta^2)]^{1/2} = 0.6785$. Although the correlation functions are not in a good exponential form because η is not close to 1, we can still see that the correlation decays very rapidly.

The three kinds of transverse correlation are given by

$$\begin{aligned}\langle S_{i,+}^A S_{j,-}^B \rangle &= \langle a_{i\uparrow}^\dagger a_{i\downarrow} b_{j\downarrow}^\dagger b_{j\uparrow} \rangle \\ &= -|g(R_{ij})|^2 \\ &\quad - (S^B - S^A) g(R_{ij}) \sinh 2\theta_k|_{k=0}, \end{aligned} \tag{16a}$$

$$\begin{aligned}\langle S_{i,+}^A S_{j,-}^A \rangle &= \langle a_{i\uparrow}^\dagger a_{i\downarrow} a_{j\downarrow}^\dagger a_{j\uparrow} \rangle \\ &= |f(R_{ij})|^2 \\ &\quad + 2(S^B - S^A) f(R_{ij}) \sinh^2 \theta_k|_{k=0}, \end{aligned} \tag{16b}$$

$$\begin{aligned}\langle S_{i,+}^B S_{j,-}^B \rangle &= \langle b_{i\uparrow}^\dagger b_{i\downarrow} b_{j\downarrow}^\dagger b_{j\uparrow} \rangle \\ &= |f(R_{ij})|^2 \\ &\quad + 2(S^B - S^A) f(R_{ij}) \cosh^2 \theta_k|_{k=0}. \end{aligned} \tag{16c}$$

We note that the transverse correlation length is two times the longitudinal one. The SWT calculation gives that the longitudinal correlation length $\xi = 1/(2\ln 2) = 0.7213$,[2] while the numerical methods cannot give the accurate correlation length, because the fluctuation decays so rapidly.

IV. THERMODYNAMIC PROPERTIES AT FINITE TEMPERATURES

We investigate the low-temperature asymptotic expansion of the self-consistent equations (11) and verify that it changes continuously into Eqs. (12) in $T=0$ K. Equation (11a) has a solution for $T \neq 0$ K. So there is no boson condensation. Equation (11a) gives the gap of the ferromagnetic branch as

$$\Delta_{\mathrm{ferro}} = \frac{\sqrt{1-\eta^2}}{\eta^2} \frac{2T^2}{(S^B - S^A)^2 \Lambda_1} \approx 2.4436 T^2.$$

We solved the self-consistent equations (11) numerically and find that the values of the variation parameters are continuously evolved to the values at $T=0$ K. On the other hand, we see that the mean-field theory fails and the bond operator D is zero when T is higher than a specific temperature, say, approximately 1.38 in our case. The failure of the mean field indicates that the system has entered a local-moment phase in which there is no correlation of the spin fluctuation, as pointed out by Arovas and Auerbach.[9] With temperature increasing, we find that the gap of the antiferro-

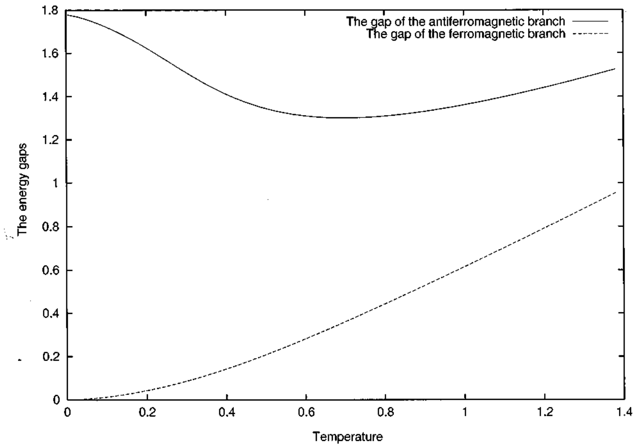

FIG. 1. The gaps of the ferromagnetic and antiferromagnetic branches.

magnetic branch $\Delta_{anti}=\Lambda_2+\Lambda_1\sqrt{1-\eta^2}$ varies. In the temperature region where the SBMFT is valid, this gap first decreases and then increases. It reaches its minimum, which is about 1.30 when $T\approx 0.7$. The gaps of the ferromagnetic and antiferromagnetic branches are plotted in Fig. 1. And the free energy versus T is calculated and plotted in Fig. 2 with the argument of dividing the part of fluctuation by 2.[9,10]

The spin correlations at $T\rightarrow 0$ K are calculated:

$$\langle \vec{S}_i^A\cdot\vec{S}_j^B\rangle=-\frac{3}{2}|G(R_{ij})|^2,$$

$$G(R_{ij})=\frac{1}{2}\int_{-\pi/2}^{\pi/2}\frac{dk}{2\pi}\sinh 2\theta_k\left\{\coth\frac{\beta}{2}E_k^\alpha+\coth\frac{\beta}{2}E_k^\beta\right\}\times e^{-ikR_{ij}}, \tag{17a}$$

$$\langle \vec{S}_i^A\cdot\vec{S}_j^A\rangle=\frac{3}{2}|F_1(R_{ij})|^2,$$

$$F_1(R_{ij})=\int_{-\pi/2}^{\pi/2}\frac{dk}{2\pi}\left\{\cosh^2\theta_k\coth\frac{\beta}{2}E_k^\alpha+\sinh^2\theta_k\coth\frac{\beta}{2}E_k^\beta\right\}e^{-ikR_{ij}}, \tag{17b}$$

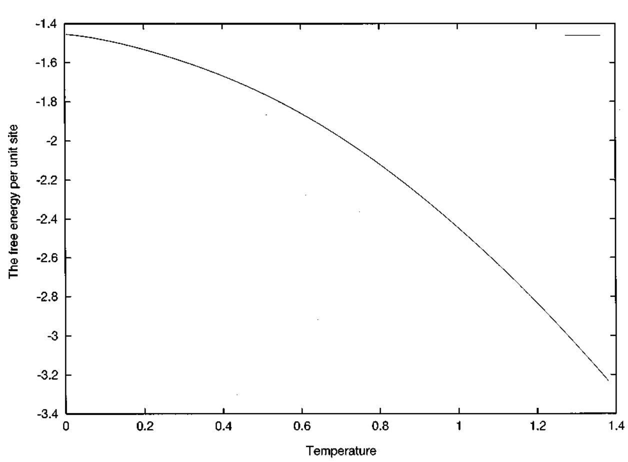

FIG. 2. The free energy F versus T.

$$\langle \vec{S}_i^B\cdot\vec{S}_j^B\rangle=\frac{3}{2}|F_2(R_{ij})|^2,$$

$$F_2(R_{ij})=\int_{-\pi/2}^{\pi/2}\frac{dk}{2\pi}\left\{\sinh^2\theta_k\coth\frac{\beta}{2}E_k^\alpha+\cosh^2\theta_k\coth\frac{\beta}{2}E_k^\beta\right\}e^{-ikR_{ij}}. \tag{17c}$$

Because Δ_{ferro} behaves as T^2, the correlation length behaves as T^{-1}, i.e., $\xi=\eta^2\Lambda_1(S^B-S^A)/(4\sqrt{1-\eta^2})T^{-1}$.

The dynamic magnetic susceptibility is calculated by using linear-response theory,

$$\begin{pmatrix}\Delta S_z^A(q,\omega)\\ \Delta S_z^A(q,\omega)\end{pmatrix}=-g\begin{pmatrix}\langle\langle S_z^A S_z^A\rangle\rangle_{q\omega} & \langle\langle S_z^A S_z^B\rangle\rangle_{q\omega}\\ \langle\langle S_z^B S_z^A\rangle\rangle_{q\omega} & \langle\langle S_z^B S_z^B\rangle\rangle_{q\omega}\end{pmatrix}\times\begin{pmatrix}h_A(q,\omega)\\ h_B(q,\omega)\end{pmatrix}, \tag{18}$$

where $\langle\langle S_z^A S_z^A\rangle\rangle$, etc., is the retarded Green function, and h_A, h_B are the small external magnetic field, and g is the Laude factor. In the Matsubra representation, the dynamic magnetic susceptibilities are given by

$$\begin{aligned}\chi_{AA}^{zz}(q,i\omega_n)&=-g^2\langle\langle S_z^A S_z^A\rangle\rangle_{q\omega}\\ &=\frac{g^2}{2N}\sum_k\left\{\frac{n_B(E_k^\alpha)-n_B(E_{k+q}^\alpha)}{i\omega_n+E_{k+q}^\alpha-E_k^\alpha}\times\cosh^2\theta_{k+q}\cosh^2\theta_k\right.\\ &\quad+\frac{n_B(E_{k+q}^\beta)-n_B(E_q^\beta)}{i\omega_n-E_{k+q}^\beta+E_k^\beta}\sinh^2\theta_{k+q}\sinh^2\theta_k\\ &\quad+\frac{1+n_B(E_k^\beta)+n_B(E_{k+q}^\alpha)}{i\omega_n+E_{k+q}^\alpha+E_k^\beta}\cosh^2\theta_{k+q}\sinh^2\theta_k\\ &\quad\left.-\frac{1+n_B(E_k^\alpha)+n_B(E_{k+q}^\beta)}{i\omega_n-E_{k+q}^\beta-E_k^\alpha}\cosh^2\theta_k\sinh^2\theta_{k+q}\right\},\end{aligned} \tag{19a}$$

$$\begin{aligned}\chi_{AB}^{zz}(q,i\omega_n)&=-g^2\langle\langle S_z^A S_z^B\rangle\rangle_{q\omega}\\ &=\frac{g^2}{2N}\sum_k\sinh\theta_k\sinh\theta_{k+q}\cosh\theta_k\cosh\theta_{k+q}\\ &\quad\times\left\{\frac{1+n_B(E_{k+q}^\beta)+n_B(E_k^\alpha)}{i\omega_n-E_{k+q}^\beta-E_k^\alpha}\right.\\ &\quad+\frac{n_B(E_{k+q}^\alpha)-n_B(E_k^\alpha)}{i\omega_n+E_{k+q}^\alpha-E_k^\alpha}+\frac{n_B(E_k^\beta)-n_B(E_{k+q}^\beta)}{i\omega_n+E_k^\beta-E_{k+q}^\beta}\\ &\quad\left.-\frac{1+n_B(E_{k+q}^\alpha)+n_B(E_k^\beta)}{i\omega_n+E_{k+q}^\alpha+E_k^\beta}\right\}.\end{aligned} \tag{19b}$$

$\chi_{BB}^{zz}(q,i\omega_n)$ and $\chi_{BA}^{zz}(q,i\omega_n)$ can be obtained by the exchange $(\alpha\leftrightarrow\beta)$ in Eqs. (19a) and (19b), respectively.

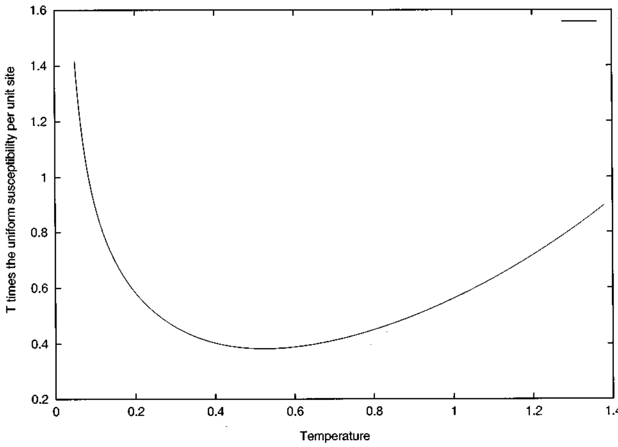

FIG. 3. The $T\chi_{uni}/Ng^2$ versus T.

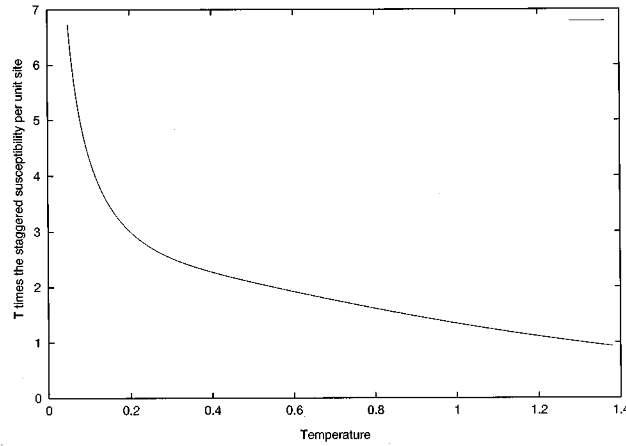

FIG. 4. The $T\chi_{stag}/Ng^2$ versus T.

The mean-field static uniform and staggered magnetic susceptibilities per unit cell are

$$\frac{\chi_{uni}^{MF}}{N}=g^2\beta\int_{-\pi/2}^{\pi/2}\frac{dk}{2\pi}\{n_k^{\alpha}(n_k^{\alpha}+1)+n_k^{\beta}(n_k^{\beta}+1)\}, \quad (20a)$$

$$\frac{\chi_{stag}^{MF}}{N}=g^2\beta\int_{-\pi/2}^{\pi/2}\frac{dk}{2\pi}\left\{[n_k^{\alpha}(n_k^{\alpha}+1)+n_k^{\beta}(n_k^{\beta}+1)]\cosh^2 2\theta_k + 2\sinh^2 2\theta_k\frac{1+n_k^{\alpha}+n_k^{\beta}}{\beta(E_k^{\alpha}+E_k^{\beta})}\right\}. \quad (20b)$$

If $S^A=S^B$, the above equations are reduced to the familiar forms of the antiferromagnetic case,[9] which are

$$\frac{\chi_{uni}^{MF}}{2N}=g^2\beta\int_{-\pi/2}^{\pi/2}\frac{dk}{2\pi}n_k(n_k+1), \quad (20c)$$

$$\frac{\chi_{stagger}^{MF}}{2N}=g^2\beta\int_{-\pi/2}^{\pi/2}\frac{dk}{2\pi}\left\{n_k(n_k+1)\cosh^2 2\theta_k + \frac{n_k^{\beta}+1/2}{\beta E_k^{\beta}}\sinh^2 2\theta_k\right\}. \quad (20d)$$

For low temperatures, both χ_{uni}^{MF} and χ_{stag}^{MF} are proportional to T^{-2}, e.g., $\chi_{uni}^{MF}=g^2\Lambda_1\eta^2(S^B-S^A)^3/(2\sqrt{(1-\eta^2)})T^{-2}$, and so on. We plot $T\chi_{uni}/Ng^2$ versus T in Fig. 3 and $T\chi_{stag}/Ng^2$ versus T in Fig. 4. There we have multiply the mean-field susceptibilities with the factor $\frac{2}{3}$ due to the same argument as Arovas and Auerbach.[9,10] $T\chi_{uni}/Ng^2$ reaches a minimum of 0.4 at the intermediate-temperature region around $T\approx 0.5$. This is due to the contribution from the gapful antiferromagnetic branch. The low-temperature behavior of $T\chi_{uni}/Ng^2$ when $T<0.4-0.5$, the location, and the value of the minimum are found in good agreement with the QMC and DMRG calculations, even better than the MSWT calculation with improved dispersion relations.[6] After the point of minimum, the SBMFT result increases too rapidly, showing a discrepancy with numerical calculations. $T\chi_{stag}/Ng^2$ is dropped rapidly and monotonously with the temperature increasing.

The specific heat C/N versus T is calculated by the numerical differentiation of the internal energy with T, and is plotted in Fig. 5. We also find the low-temperature behavior of $C\propto T^{1/2}$, which agrees with the QMC and DMRG calculation[5,6] well when $T<0.4$. Again the SBMFT result increases rapidly, failing to see the Schottky-like peak[6] at intermediate temperatures.

In short, the SBMFT result describes the thermodynamic properties well at low temperatures ($T<0.4$–0.5). The disagreement in intermediate and high temperatures is also owing to the static and uniform constraint.

V. CONCLUSIONS

Using the Schwinger-boson mean-field theory, we have investigated both the ground state and the thermodynamic properties of the Heisenberg ferrimagnetic spin chain. The long-range ferrimagnetic order of the ground state is caused by the condensation of the Schwinger bosons. The spin fluctuations to the ground state are anisotropic and decays very rapidly. The excitation spectrum has both the low-energy ferromagnetic branch that is gapless at $T=0$ K and the high-energy antiferromagnetic branch with a gap is 1.778 at $T=0$ K. With the temperature increasing, the branch of the ferromagnetic become gapful. Δ_{ferro} behaves as T^2 and Δ_{anti} varies. At low temperatures, the ferrimagnetic spin chain exhibits the feature of the ferromagnetism. The static magnetic susceptibility, the spin-correlation length, and the specific heat behave as T^{-2}, T^{-1}, and $T^{1/2}$, respectively. At

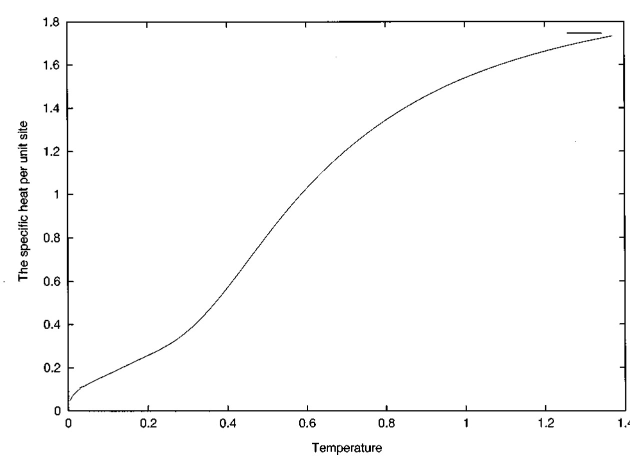

FIG. 5. The specific heat versus T.

intermediate temperatures, the antiferromagnetic branch begins to play an important role.[6] The $T\chi_{uni}$ has a minimum at $T\approx 0.5$.

Compared with other approaches, the SBMFT is a simple mean-field theory but can give many good results at both zero and finite temperatures. The spin reduction and gap of the antiferromagnetic branch Δ_{anti} at $T=0$ K differ from the numerical calculations less than 1%. The thermodynamic properties, such as the static uniform magnetic susceptibility χ_{uni} and the specific heat C calculated by the SBMFT, agree with numerical results well when $T<0.4$. The spin correlation that is anisotropic at the ground state and isotropic at finite temperatures can be calculated easily. These results improve those of the SWT (Ref. 2) largely and are consistent with those of the more complicated MSWT and numerical methods.[5,6]

The SBMFT is not successful at intermediate and high temperatures. The behavior of χ_{uni} has quantitative discrepancy with numerical results, and that of C does not agree with numerical calculations qualitatively when $T>0.4$. Both of them increase too rapidly with temperatures increasing. When $T>1.38$, the order parameter drops to zero and the SBMFT theory fails. It cannot describe the system in the whole temperature range as the numerical methods and the MSWT do.

ACKNOWLEDGMENTS

We thank Professor Tian Guangshan for his stimulating remarks.

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