

Thermodynamic properties of one-dimensional spin-1 antiferromagnetic Heisenberg chains: Green's-function approach

Shu-Qing Bao, Hu Zhao, Jue-Lian Shen, and Guo-Zhen Yang

Institute of Physics, Chinese Academy of Sciences, Beijing 100080, People's Republic of China

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The one-dimensional spin-1 Heisenberg antiferromagnetic chains are studied by a generalized two-time Green's-function method at finite temperature. $\langle S_i^z \rangle$ is set to zero at each site to guarantee the lack of the long-range order in the one-dimensional Heisenberg system. The Green's functions are decoupled in terms of the correlation functions of spin operators. A set of self-consistent equations of the correlation functions are derived and solved numerically. Correlation functions of spin operators, thermodynamic properties such as the internal energy, and specific heat in the entire temperature region are obtained. The Haldane gap in the excitation spectrum appears naturally in the analytical result. When k is zero, there is a gap 2Δ , which is $1.0J$ and close to the theoretical result of White and Huse. And there is a broad maximum in the temperature dependence of the specific heat. The properties of the thermodynamic quantities are consistent with the numerical results on the finite chains.

I. INTRODUCTION

Haldane predicted¹ in 1983 that the integer spin antiferromagnetic Heisenberg chain has a unique disordered ground state and a finite excitation gap. This conjecture has been checked experimentally,² especially with the compound NENP [$\text{Ni}(\text{C}_2\text{H}_8\text{N}_2)_2\text{NO}_2\text{ClO}_4$] for which inelastic neutron scattering and susceptibility measurements have clearly shown the existence of a spin gap.³ Recently, besides the usual Haldane systems, such as CsNiCl_3 , NENP, and AgVP_2S_6 , Y_2BaNiO_5 is also found as a new Haldane state compound and this system can be described by a one-dimensional (1D) Hamiltonian with exchange anisotropy ($J_z \neq J_{x,y}$) or planar anisotropy.⁴ Haldane's conjecture is also confirmed theoretically.^{5,7} In particular, White and Huse,⁶ who developed the density-matrix renormalization-group techniques, have calculated a variety of properties of the Heisenberg chain and got important results. The ground-state energy and Haldane gap are found to be $e_0 = -1.401\,484\,038\,971(4)$ and $\Delta = 0.410\,50(2)$. About the excitation spectrum, they found that, at $k \geq 0.3\pi$, the lowest stable excitation can be well described by the one-magnon excitation, while at small momentum the excitation spectrum is governed by the multimagnon excitation where the single magnon is unstable to decay into two magnons and the lowest stable excitation is that of the two magnon. The Haldane gap occurs at $k = \pi$ and the gap at $k = 0$ is two times the gap at $k = \pi$. This is also obtained by Takahashi.^{5,7} Affleck, Kennedy, Lieb, and Tasaki⁸ have introduced an exactly solvable model with the Hamiltonian $H = \sum_i [\mathbf{S}_i \mathbf{S}_{i+1} + \beta(\mathbf{S}_i \mathbf{S}_{i+1})^2]$, ($\beta = -\frac{1}{3}$). The ground state is constructed out of valence bonds. Such a model has the typical nature predicted by Haldane. Affleck and Lieb also made clear the difference between integer spin and half-integer spin systems and the origin of the gap.

Haldane's conjecture has also stimulated a lot of attention on the thermodynamic properties of the 1D spin-1 antiferromagnetic Heisenberg chains. Actually, long before Haldane's

conjecture, De Neef and Blöte^{9,10} had calculated the specific heat of magnetic linear chains for spin-1 and other spins by a numerical diagonalization method. Later, some others discussed the same problems^{11,12} numerically. Among them, Yamamoto and Miyashita¹² have recently investigated the low-temperature behavior of thermodynamic quantities in 1D spin-1 isotropic antiferromagnetic Heisenberg chains by a quantum Monte Carlo method. Their results show that the specific heat is linear at the low-temperature region and exhibits a broad maximum at the intermediate temperature.

However, until now few studies have been done on the excitation spectrum and the thermodynamic properties of the spin-1 Haldane systems by the two-time Green's-function method. The original two-time Green's-function method introduced by Tyablibov¹³ is very successful in the study of three-dimensional magnetic systems in which the long-range order exists. The decoupling procedure gives a spin-wave spectrum which depends on $\langle S_i^z \rangle$. Since $\langle S_i^z \rangle$ vanishes in one dimension, Kondo and Yamaji,¹⁴ proposed a new decoupling at a stage one step further than Tyablibov. Thus $\langle S_i^z \rangle = 0$ is satisfied at each site and the Green's functions are expressed in terms of correlations. By this method, Kondo and Yamaji have studied the spin- $\frac{1}{2}$ isotropic Heisenberg chains. Their results are consistent with the numerical calculation of finite chains by Bonner and Fisher.¹⁵ The nearly same method was also used by Richards,¹⁶ Scales and Gersch,¹⁷ Rhodes and Scales¹⁸ to study one-dimensional Heisenberg chains. Such a method was called the second-order Green's-function method in these papers. However, their excitation energy for integer spins has a zero gap at $k = 0$. The Haldane gap is also discussed by the spin-wave theory.¹⁹ However, the excitation spectrum has a gap Δ at $k = 0$ which deviates from the result 2Δ by White and Huse⁶ and Takahashi.⁷

In the present work, we generalize Kondo and Yamaji's decoupling technique of Green's-function method for the spin- $\frac{1}{2}$ isotropic Heisenberg chains to the 1D spin-1 antiferromagnetic Heisenberg chains. We do not use the concept of sublattice that appeared in the spin-wave theory¹⁹ because of

the disordered ground state of spin-1 systems. $\langle S_i^z \rangle$ is set equal to zero at each site. The Green's functions are expressed in terms of the correlations $\langle S_0^z S_n^z \rangle$ and $\langle S_0^+ S_n^- \rangle$ which are determined by a set of self-consistent equations. A new decoupling approximation has been introduced which is different from Refs. 16–18 and a new formula of the excitation spectrum can be obtained from the analytical results. At $k=0$ in our excitation spectrum, there is a gap 2Δ which equals $1.0J$. This result is close to the exact numerical results of White and Huse⁶ and Takahashi.⁷ Our results at small k are better than that of Refs. 16–18 and that of spin-wave theory.¹⁹ However, the value of gap at larger k in our results deviates from that of White and Huse⁶ and that of the spin wave theory.²⁰ We believe this is the flaw of the decoupling approximation in the Green's-function method. But the thermodynamic quantities in the whole temperature range can be obtained by this method. In the present work thermodynamic properties such as the internal energy and specific heat at arbitrary temperature are obtained after solving the set of self-consistent equations numerically. There is a broad maximum in the curve of the temperature dependence of the specific heat. These results are consistent with the numerical results of Yamamoto and Miyashita¹² and the experimental results.¹¹

Section II gives the formalism of the generalized two-time Green's-function method and the final set of equations of correlation functions. Section III provides numerical solutions and discussion. The final section is a summary.

II. GENERALIZED TWO-TIME GREEN'S-FUNCTION METHOD

The 1D spin-1 antiferromagnetic Heisenberg chain with both exchange anisotropy and single-ion anisotropy can be expressed by the Hamiltonian

$$H = J \sum_{i=-N/2+1}^{N/2} \left[S_i^z S_{i+1}^z + \frac{\gamma}{2} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) \right] + D \sum_{i=-N/2+1}^{N/2} (S_i^z)^2, \quad (1)$$

where $J > 0$ is considered. S_i^x , S_i^y , and S_i^z represent the three components of the spin-1 operator at site i with $S_i^\pm = S_i^x \pm iS_i^y$. γ is the exchange anisotropic parameter and D is the single-ion anisotropic parameter. When $D=0, \gamma=1$, Eq. (1) changes into the isotropic Heisenberg model. We will begin with the formalism of the two-time Green's function whose time-Fourier transform satisfies the equation

$$\omega \langle \langle A; B \rangle \rangle = (2\pi)^{-1} \langle [A, B] \rangle + \langle \langle [A, B]; B \rangle \rangle, \quad (2)$$

where $[A, B]$ denotes the commutator of the two operators A and B and $\langle \langle A; B \rangle \rangle$ is the time-Fourier transformation of the Green function $G_{AB}(t)$ of the two operators A and B :

$$\langle \langle A; B \rangle \rangle = \frac{1}{2\pi} \int_{-\infty}^{+\infty} G_{AB}(t) e^{i\omega t} dt, \quad (3)$$

$$G_{AB}(t) = -i\theta(t) \langle [A, B] \rangle, \quad (4)$$

$\theta(t)$ is the step function of time, $\langle \dots \rangle$ denotes the thermal average which is given by

$$\langle BA \rangle = i \int_{-\infty}^{+\infty} d\omega [\langle \langle A; B \rangle \rangle_{\omega+i\delta} - \langle \langle A; B \rangle \rangle_{\omega-i\delta}] n(\beta\omega), \quad (5)$$

where $n(x) = 1/[\exp(x) - 1]$, $\beta = 1/k_B T$, k_B is the Boltzmann constant. We first consider the Green's function $\langle \langle S_0^z; S_n^z \rangle \rangle$. Using the formalism (2), we get

$$\omega \langle \langle S_0^z; S_n^z \rangle \rangle = \frac{J}{2} \gamma \langle \langle S_0^+ S_1^- - S_{-1}^+ S_0^- - S_0^- S_1^+ + S_{-1}^- S_0^+; S_n^z \rangle \rangle. \quad (6)$$

Furthermore, after a similar calculation, the equations of motion for the Green's functions on the right-hand side of the above equation can be obtained easily. For example, the equation of motion of the Green's function $\langle \langle S_0^+ S_1^-; S_n^z \rangle \rangle$ is

$$\begin{aligned} (\omega - J + 2JD') \langle \langle S_0^+ S_1^-; S_n^z \rangle \rangle &= \frac{1}{2\pi} (-\delta_{0n} + \delta_{1n}) \langle S_0^+ S_1^- \rangle + 2J \gamma \langle \langle S_0^z - S_1^z; S_n^z \rangle \rangle \\ &+ J \langle \langle -S_0^+ S_1^- S_1^z - S_{-1}^z S_0^+ S_1^- + \gamma S_{-1}^+ S_0^z S_1^- - \gamma S_0^z S_1^z S_1^z - 2D' S_0^+ S_0^z S_1^-; S_n^z \rangle \rangle \\ &+ J \langle \langle S_0^+ S_1^- S_2^z + S_0^+ S_0^z S_1^- - \gamma S_0^+ S_1^z S_2^z + \gamma S_1^z S_0^z S_2^z + 2D' S_0^+ S_1^- S_1^z; S_n^z \rangle \rangle, \end{aligned} \quad (7)$$

where we have let $JD' = D$ for convenience and we have used the commutation relations of spin operators, such as $S_i^z S_i^- - S_i^- S_i^z = -S_i^-$ and the special property of the $S=1$ operators

$$S_i^- S_i^+ = 2 - S_i^z - (S_i^z)^2, \quad (8)$$

where i refers to an arbitrary lattice site.

It should be emphasized that all results obtained above are exact. We have not made any approximation. The term $-J + 2JD'$ in the coefficient of the Green's function $\langle \langle S_0^+ S_1^-; S_n^z \rangle \rangle$ in the left-hand side of Eq. (7) is obtained from the commutation relations of spin-1 operators. While using Eq. (2) to calculate the equation of motion of the Green's function $\langle \langle S_0^+ S_1^-; S_n^z \rangle \rangle$, for example, we have a

further higher-order Green's function of the four-operator $J\langle\langle -S_0^+ S_1^- S_1^z; S_n^z \rangle\rangle$ which equals to $-J\langle\langle S_0^+ S_1^- S_1^z; S_n^z \rangle\rangle + J\langle\langle S_0^+ S_1^-; S_n^z \rangle\rangle$. The last term is just the second term on the left-hand side of Eqs. (7) and the first term will be decoupled together with other Green's functions on the right-hand side of Eq. (7). Later we will see that it is the J that is responsible for the Haldane gap. So the Haldane gap arises naturally in the generalized Green's-function method and its value predicted by this method is analytical. However, our result is different with that of Ref. 18 where the decoupling approximation has been made earlier in Eq. (3.1) of Ref. 18. Thus it is this key difference that causes our results to differ from those of Refs. 16–18. At the same time, it is also interesting to note that the term responsible for the Haldane gap in spin-1 Heisenberg chains does not appear in the corresponding equation of the spin- $\frac{1}{2}$ isotropic Heisenberg chains¹⁴ because of the relations such as $2S_i^+ S_i^z = -S_i^+$, and $2S_i^z S_i^- = -S_i^-$ for spin- $\frac{1}{2}$ operators. Therefore the following two terms $\langle\langle S_0^+ S_0^z S_1^-; S_n^z \rangle\rangle$ and $-\langle\langle S_0^+ S_1^- S_1^z; S_n^z \rangle\rangle$ are canceled out by each other, so that there is no gap at $k=0$ for the spin- $\frac{1}{2}$ isotropic Heisenberg chains.¹⁴ This implies that the generalized two-time Green's-function method can explain the different behavior of spin-1 and spin- $\frac{1}{2}$ at small k .

Similarly we can get equations of motion of other Green's-functions in the right-hand side of Eq. (6). We decouple the Green's function on the right-hand side of Eq. (7) by the following rules:

$$\langle\langle S_0^+ S_1^- S_1^z; S_n^z \rangle\rangle \rightarrow \alpha_1 \langle S_0^+ S_1^- \rangle \langle\langle S_1^z; S_n^z \rangle\rangle, \quad (9)$$

$$\begin{aligned} \langle\langle S_0^z S_0^z S_1^z; S_n^z \rangle\rangle &\rightarrow \alpha_2 \langle S_0^z S_0^z \rangle \langle\langle S_1^z; S_n^z \rangle\rangle \\ &+ \alpha_2 \langle S_0^z S_1^z \rangle \langle\langle S_0^z; S_n^z \rangle\rangle, \end{aligned} \quad (10)$$

where we have introduced two parameters α_1 and α_2 because of the exchange anisotropy, and $\alpha_1 = \alpha_2$ when $\gamma = 1$. In this work, for simplicity we use the same α_1 and α_2 whenever the corresponding decouplings are introduced.

After defining C_n by $C_n^z = \alpha_1 \langle S_0^z S_n^z \rangle$ and $C_n^\pm = \alpha_2 \langle S_0^+ S_n^- \rangle$ with $n=0,1,2,\dots$, Eq. (6) becomes

$$\begin{aligned} (\omega - J + 2JD')\omega \langle\langle S_0^z; S_n^z \rangle\rangle &= \frac{J}{2} \gamma \left\{ \frac{1}{2\pi} D_n + B_0 \langle\langle S_0^z; S_n^z \rangle\rangle \right. \\ &+ B_1 \langle\langle S_1^z + S_{-1}^z; S_n^z \rangle\rangle \\ &\left. + B_2 \langle\langle S_2^z + S_{-2}^z; S_n^z \rangle\rangle \right\}, \end{aligned} \quad (11)$$

where

$$D_n = (-4\delta_{0n} + 2\delta_{1n} + 2\delta_{-1n}) \langle S_0^+ S_1^- \rangle,$$

$$B_0 = 4J[2\gamma - \gamma C_0^z + 2\gamma C_1^z + (1 - 2D')C_1^\pm + \gamma C_2^\pm],$$

$$B_1 = 2J[-2\gamma + \gamma C_0^z - 2\gamma C_1^z - 2(1 - D')C_1^\pm - \gamma C_2^\pm],$$

$$B_2 = 2JC_1^\pm.$$

The Fourier transformation of $\langle\langle S_0^z; S_n^z \rangle\rangle$ is defined as

$$G'(k, \omega) = \sum_n e^{ikna} \langle\langle S_0^z; S_n^z \rangle\rangle, \quad (12)$$

where a is the lattice spacing and will be set to 1 in this work. Then from Eq. (11) and Eq. (12) we get

$$G'(k, \omega) = \frac{P_k/2}{(\omega - \Omega_{k1})(\omega - \Omega_{k2})}, \quad (13)$$

where

$$P_k = 2J\gamma(-1 + \cos k) \langle S_0^+ S_1^- \rangle / \pi, \quad (14)$$

and

$$\begin{aligned} \Omega_{k1,2}/J &= \frac{1}{2}(1 - 2D') \pm \frac{1}{2} \{ (1 - 2D')^2 \\ &+ 2\gamma(B_0 + 2B_1 \cos k + 2B_2 \cos 2k)/J \}^{1/2}. \end{aligned} \quad (15)$$

Then the correlation $\langle S_n^z S_0^z \rangle$ can be obtained by using Eq. (5). We have

$$\langle S_n^z S_0^z \rangle = \frac{\pi}{N} \sum_k e^{-ikn} \frac{P_k}{\Omega_{k1} - \Omega_{k2}} [n(\beta\Omega_{k1}) - n(\beta\Omega_{k2})]. \quad (16)$$

If $D=0$, Eq. (15) can be simplified as

$$\begin{aligned} \Omega_{k1,2}/J &= \frac{1}{2} \pm \frac{1}{2} \{ 1 + 8\gamma(2\gamma - \gamma C_0^z + 2\gamma C_1^z + \gamma C_2^\pm \\ &- 2C_1^\pm \cos k)(1 - \cos k) \}^{1/2}. \end{aligned} \quad (17)$$

From this equation we can see that there are two branches of the excitation spectrum. For the positive one, if $k=0$, there is a gap $1.0J$ for $D=0$. We will return to this problem in the next section.

Similarly, for the correlation $\langle S_n^+ S_0^- \rangle$, if $D=0$, we have

$$\langle S_n^+ S_0^- \rangle = \frac{1}{N} \sum_k e^{-ikn} \frac{Z_k}{\omega_{k1} - \omega_{k2}} [n(\beta\omega_{k1}) - n(\beta\omega_{k2})], \quad (18)$$

with

$$Z_k = 2J\{2(-1 + \gamma \cos k) \langle S_0^z S_1^z \rangle + (-\gamma + \cos k) \langle S_0^+ S_1^- \rangle\}, \quad (19)$$

and

$$\omega_{k1,2}/J = \frac{1}{2} \pm \frac{1}{2} \{ 1 + A_0 + 2A_1 \cos k + 2A_2 \cos 2k \}^{1/2}, \quad (20)$$

where

$$A_0 = 4\{4 + (-2 + \gamma^2)C_0^\pm + 2\gamma^2 C_1^z + 3\gamma C_1^\pm + 2C_2^z + \gamma^2 C_2^\pm\},$$

$$A_1 = 2\{-4\gamma + \gamma C_0^\pm - 4\gamma C_1^z - 2(1 + \gamma^2)C_1^\pm - 2\gamma C_2^z - \gamma C_2^\pm\},$$

$$A_2 = 2\gamma\{2\gamma C_1^z + C_1^\pm\}.$$

Equations (16) and (18) for $n=0,1,2,\dots$, together with Eq. (8), consist of a set of self-consistent equations which can be solved numerically and the correlations, internal energy, and specific heat, etc., can then be obtained.

From Eqs. (16) and (18), if $D=0, \gamma=1$, we obtain the rotational invariance of correlations: $\langle S_n^+ S_0^- \rangle = 2\langle S_n^z S_0^z \rangle$.

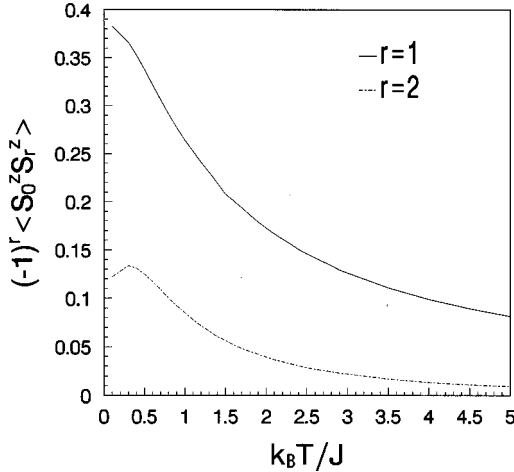


FIG. 1. Correlations $|\langle S_0^z S_1^z \rangle|$ and $\langle S_0^z S_2^z \rangle$ vs temperature for the 1D spin-1 isotropic antiferromagnetic Heisenberg chain.

This is certainly correct because of the symmetry: $z \leftrightarrow x$ and $z \leftrightarrow y$ of the isotropic Heisenberg spin chains. The results are

$$C_n^z = \frac{1}{N} \sum_k e^{-ikn} \frac{4J(-1 + \cos k) C_1^z}{\omega_{k1} - \omega_{k2}} [n(\beta \omega_{k1}) - n(\beta \omega_{k2})], \quad (21)$$

$$\omega_{k1,2}/J = \frac{1}{2} \pm \frac{1}{2} \{1 + 8(2 - C_0^z + 2C_1^z + 2C_2^z - 4C_1^z \cos k) \times (1 - \cos k)\}^{1/2}. \quad (22)$$

Here, $\alpha_1 = \alpha_2 = \alpha$, and $C_n^\pm = 2C_n^z = 2\alpha \langle S_0^z S_n^z \rangle$ because of the rotational invariance stated above. Equations (21) with $n=0,1,2$ form a set of self-consistent equations which determine the three quantities C_1^z , C_2^z , and α .

III. NUMERICAL SOLUTION AT ARBITRARY TEMPERATURE AND DISCUSSION

The set of self-consistent equations obtained in the previous section can be solved numerically by using the iteration technique at arbitrary temperature. In the present work, we only calculate the results of $D=0$ and $\gamma=1$.

We present our results of the variations of $|\langle S_0^z S_1^z \rangle|$ and $\langle S_0^z S_2^z \rangle$ with temperature in Fig. 1. The temperature dependence of $\langle S_0^z S_1^z \rangle$ from our method is in general agreement with the behavior of Fisher's classical model²¹ in the whole temperature region although the actual values are not the same. While in Ref. 18 the nearest-neighbor correlation function deviates from Fisher's result at low temperature. Our results show that as $T \rightarrow 0$, the value of the correlations tend to $\langle S_0^z S_1^z \rangle = -0.38483$ and $\langle S_0^z S_2^z \rangle = 0.11764$ which are consistent with that obtained by Takahashi²² and Liang.²³ At higher temperature, after a high-temperature expansion, we found that $\langle S_0^z S_1^z \rangle \approx -2/3 \theta$, $\langle S_0^z S_2^z \rangle \approx 1/3 \theta^2$, where $\theta = K_B T/J$. From Fig. 1, we can see that the correlations have the same behavior as that predicted by our high-temperature expansion and that $\langle S_0^z S_2^z \rangle$ tends to zero at higher temperature.

In Fig. 2, the excitation spectrum ω_k is plotted versus k/π at zero temperature. We take the positive branch ω_{k1} in

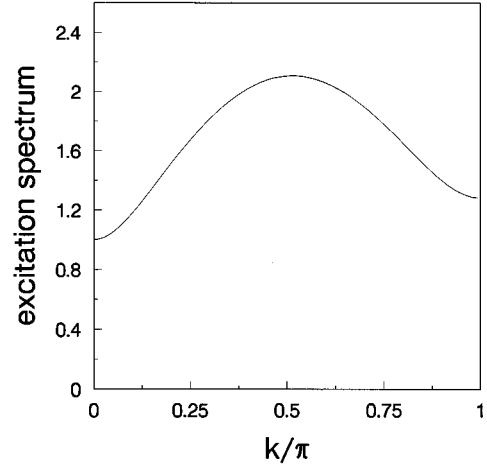


FIG. 2. The excitation spectrum ω_k vs k/π at zero temperature for the 1D spin-1 isotropic antiferromagnetic Heisenberg chain.

Eq. (22). From Fig. 2, we know that the excitation spectrum has a gap equal to 2Δ at $k=0$, $\Delta=0.5J$. This is close to the exact numerical results of White and Huse⁶ and Takahashi.⁷ Actually, in the generalized two-time Green's-function method, we have included the contributions of multimagnons as well as that of one magnon, so it is not surprising that our results at small k are quite good. This is the natural result of the generalized two-time Green's-function method. However, at larger k , our result of the value of gap deviates from the exact value. This results from the defect of the decoupling approximation in the Green's-function method which has been discussed by Kondo and Yamaji.¹⁴ However, in spin-wave theory, at $k=0$, the excitation spectrum has a gap Δ which is not consistent with the result 2Δ of White, Huse and Takahashi, while the excitation spectrum in Refs. 16–18 is $E_k^2 \propto (1 - \cos k)(1 + h \cos k)$, which is zero at $k=0$. This spectrum has the same behavior as that of the 1D spin- $\frac{1}{2}$ ferromagnetic Heisenberg chain obtained by the traditional spin-wave theory: $E_k = 2zJS(1 - \cos k)$. Actually, these papers appeared long before Haldane's conjecture. Our excitation spectrum at small k is obviously better than that obtained by spin-wave theory¹⁹ and much better than that obtained by the second-order Green's-function theory.^{16–18} (In Ref. 18, the case $J < 0$ is the antiferromagnet.)

In Fig. 3 and Fig. 4, the temperature dependences of the internal energy and the corresponding specific heat are plotted. The internal energy is defined as

$$E = \langle H \rangle = JN \{ \langle S_0^z S_1^z \rangle + \langle S_0^+ S_1^- \rangle \}. \quad (23)$$

The specific heat C is obtained by differentiating the internal energy E with respect to the temperature T . From these calculations we found that as T tends to zero, the internal energy tends to $-0.1545J$. A broad maximum exists in the curve of the specific heat versus temperature. This broad maximum occurs because we have included the "bound states" in using the decoupling procedure proposed by Kondo and Yamaji.¹⁴ The broken lines in both figures represent the numerical results obtained by Yamamoto and Miyashita¹² with the quantum Monte Carlo method, and our results are consistent with their results. We also find that our results are slightly lower than the exact numerical values.

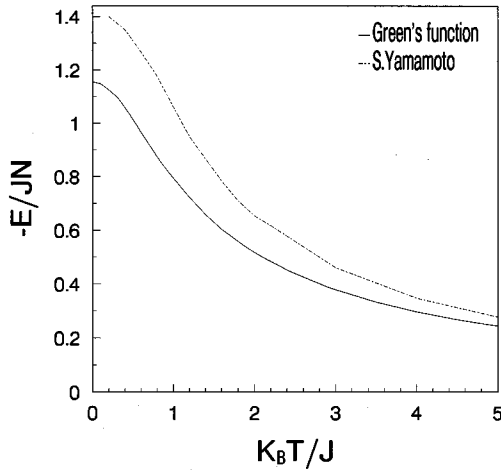


FIG. 3. Temperature dependence of the internal energy $-E/JN$ for the 1D spin-1 isotropic antiferromagnetic Heisenberg chain. The solid line represents our results obtained by the generalized two-time Green's-function method. The broken line represents Yamamoto and Miyashita's results obtained by a quantum Monte Carlo method.

IV. SUMMARY

The thermodynamic properties of the 1D spin-1 antiferromagnetic Heisenberg chains are investigated by the generalized two-time Green's-function method. $\langle S_i^z \rangle$ is set to zero at each site which guarantees the absence of long-range order in the spin-1 systems. The Green's functions are decoupled in terms of the correlations $\langle S_0^z S_n^z \rangle$ and $\langle S_0^+ S_n^- \rangle$. A set of self-consistent equations of correlations result and are solved numerically for the isotropic Heisenberg chains. Fair agreement is found in the excitation spectrum at small k mainly because we have included the contributions of the multimagnon as well as that of the one magnon. At $k=0$, the gap is found to be 2Δ which is $1.0J$ and close to the theoretical exact result of White and Huse. Thermodynamic quantities such as the internal energy and the specific heat are obtained in the wide temperature region which are found to be consistent with that obtained by the quantum Monte Carlo

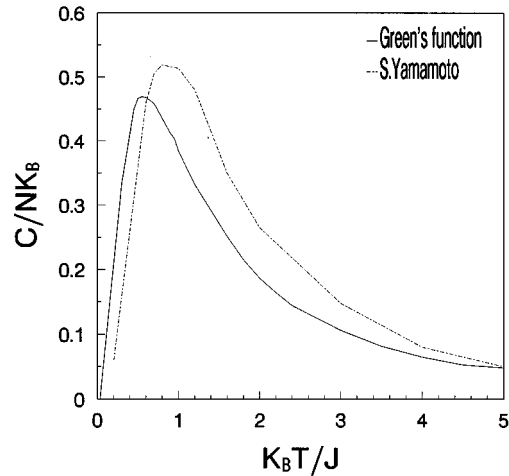


FIG. 4. Temperature dependence of the specific heat C/Nk_B for the 1D spin-1 isotropic antiferromagnetic Heisenberg chain. The solid line represents our results obtained by the generalized two-time Green's-function method. The broken line represents Yamamoto and Miyashita's results obtained by a quantum Monte Carlo method.

method. As T tends to zero, the internal energy is found to be $-0.1545J$. There is a broad maximum in the curve of the specific heat versus temperature. This result is attributed to the contribution of the "bound state" which we have included in our decoupling approximation. Finally it may be interesting to note that, with this generalized two-time Green's function method, different results at small k for spin- $\frac{1}{2}$ and spin-1 systems can be obtained which are consistent with that predicted by Haldane although the results at larger k are not satisfactory, which we should consider improving in the future. We believe that this method is still a very useful method in investigating the Heisenberg chains.

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