Signature of the Luttinger liquid phase in alternating Heisenberg spin-$\frac{1}{2}$ chains: Analytical and numerical approaches

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We have studied the zero- and low-temperature behaviors of anisotropic alternating antiferromagnetic-ferromagnetic Heisenberg spin-$\frac{1}{2}$ chains in a transverse magnetic field. Using the analytical spinless fermion approach, the thermodynamic behavior of the model has been studied. We have introduced a different order parameter to distinguish the gapless Luttinger liquid phase from the other gapped phases. The exact diagonalization Lanczos results are also used to compare with the spinless fermion ones. We have found a double peak structure in the specific-heat curves for the region between the two quantum critical points. Using the numerical full diagonalization results, the existence of the double peak structure is confirmed.

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I. INTRODUCTION

The study of continuous phase transitions has been one of the most fertile branches of theoretical physics in the last decades. Each phase can usually be characterized by an order parameter. Often, the choice of an order parameter is obvious. However, in some cases finding an appropriate order parameter is complicated. In particular, many magnetic systems experience the Luttinger liquid (LL) phase for certain values of some nonthermal control parameter. Luttinger liquid is the paradigm for the description of interacting one-dimensional (1D) quantum systems.[1,2] The correlation functions decay as power laws, and the ground state has a quasi-long-range order. In spite of all manifestations of this phase, the magnetic ordering in the LL phase is still unclear, i.e., all suggested local magnetic order parameters turn out to be zero, having no effect in determining the structure of the LL phase. In this work, we will concentrate on studying the probably nonlocal magnetic ordering of the LL phase.

One-dimensional quantum spin systems such as antiferromagnetic spin-$\frac{1}{2}$ chains,[3] spin ladder systems,[4] or bond alternating spin-$\frac{1}{2}$ antiferromagnetic-ferromagnetic (AF-F) chains are good candidates for studying the LL phase. When these systems are placed in an external magnetic field, they can be mapped onto a 1D system of interacting spinless fermions (SFs).[1,5–9] The filling of a fermionic band can thus be continuously tuned, making these systems suitable for probing the LL physics.[1,3,10,11] In the case of isotropic bond alternating AF-F spin-$\frac{1}{2}$ chains, the whole band can be covered. In the absence of an external magnetic field ($h=0$), the model is mapped onto a nonlinear sigma model with a $4\pi s$ topological angle.[12] This model is always gapful and can be regarded as a Haldane gapped spin-1 chain.[13] The gap decreases by increasing the magnetic field and goes to zero at the lower critical field h_{c_1}.[14] At h_{c_1}, the system enters the gapless phase and the fermionic band starts to be filled. This process continues until the upper critical field h_{c_2} is reached. Increasing the field beyond h_{c_2} reopens the gap and the band is then completely filled.

Recently, it was demonstrated that $CuBr_4(C_5H_{12}N)_2$ is a unique system for controlling and probing the physics of LL.[15] This sample is a spin ladder system with $h_{c_1}=6.6$ T and $h_{c_2}=14.6$ T.[16] Bond alternating AF-F spin-$\frac{1}{2}$ chains that allow experimental access to the whole fermionic band are not known. However the $(CH_3)_2NH_2CuCl_3$ system has been considered as a suitable realization of bond alternating AF-F spin chain. Linked-cluster calculations and bulk measurements show that $DMACuCl_3$ is also a realization of the spin-$\frac{1}{2}$ alternating AF-F chain with nearly the same strength of antiferromagnetic and ferromagnetic couplings.[17] Other experimental samples of the AF-F alternating spin-$\frac{1}{2}$ chain compounds have also been reported in Refs. 18–22. Although it is not known whether these systems can experience the LL phase, theoretically, an isotropic bond alternating AF-F spin chain, in its ground state, can enter the LL phase with quasi-long-range order. In this paper, we look for an order parameter to describe the LL phase of the bond alternating AF-F spin-$\frac{1}{2}$ chain. The Hamiltonian of this model with anisotropic ferromagnetic coupling is given by

$$\hat{H} = -J_{\mathrm{F}}\sum_{j=1}^{N/2}\left(S_{2j}^{x}S_{2j+1}^{x} + \Delta S_{2j}^{y}S_{2j+1}^{y} + S_{2j}^{z}S_{2j+1}^{z}\right) + J_{\mathrm{AF}}\sum_{j=1}^{N/2}\mathbf{S}_{2j-1}\cdot\mathbf{S}_{2j} + h\sum_{j=1}^{N}S_{j}^{\alpha}, \tag{1}$$

where $S_j^{\alpha},(\alpha=x,y,z)$ are spin-$\frac{1}{2}$ operators on the jth site. J_{F} and J_{AF} denote the ferromagnetic and antiferromagnetic couplings, respectively. Δ is the anisotropy parameter, and h is a uniform magnetic field.

The ground-state properties[23–29] and low-lying excitations[30] of this model have been thoroughly investigated by numerical tools and variational schemes. In particular, the string order parameter which was originally defined for the spin-1 Heisenberg chains[31] has been generalized to this system. The ground state has long-range string order, which is characteristic of the Haldane phase. Hida[32] showed that the Haldane phase of the AF-F alternating chain is stable against any strength of randomness. The ground-state phase diagram of the AF-F alternating chain in a longitudinal ($\alpha=y$) mag-

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netic field is studied using numerical diagonalization and finite-size scaling based on conformal field theory.[26] It is shown that the magnetic state is gapless and is described by the LL phase. The model represented by the Hamiltonian in Eq. (1) which includes a transverse magnetic field has been studied recently using the numerical Lanczos method.[14] The main attention of this study was focused on the investigation of field-induced effects in the ground-state phase diagram, which are present when the antiferromagnetic coupling J_{AF} dominates ($J_{\mathrm{AF}} > J_{\mathrm{F}}$). The system has two critical fields, and the energy gap in the intermediate region depends on the anisotropic parameter Δ. For $\Delta \neq 1$, the intermediate state is gapful and the ground state of the model has stripe-antiferromagnetic order.[14]

In this paper we consider again an anisotropic AF-F chain in a transverse magnetic field. Using the numerical exact diagonalization method and the analytical spinless fermion approach, we investigate the zero-temperature and thermodynamic behaviors of the model. We introduce a different mean-field order parameter which can distinguish the LL phase from the other gapped phases (Fig. 2). In the specific-heat curves versus temperature, a double peak structure appears in the intermediate region of the magnetic fields $h_{c_1} < h < h_{c_2}$.

The outline of this paper is as follows. In Sec. II we discuss the zero-temperature ground-state phase diagram of the model. In Sec. III we present the results of the spinless fermion approach and the numerical full diagonalization (FD) results on the low-temperature behavior of the model. Finally we conclude and summarize our results in Sec. IV.

II. ZERO-TEMPERATURE BEHAVIOR

A. Results from the numerical Lanczos method

In this section we briefly discuss model (1) in the limiting case of the strong AF coupling $J_{\mathrm{AF}} \gg J_{\mathrm{F}}$. In this limit the model can be mapped onto an effective spin-chain Hamiltonian.[33] At $J_{\mathrm{AF}} \gg J_{\mathrm{F}}$, the system behaves as a nearly independent block of pairs.[33] Indeed an individual block may be in a singlet or a triplet state with the corresponding energies given by

$$E_{1,-1} = \frac{J_{\mathrm{AF}}}{4} \mp h, \quad E_0 = \frac{J_{\mathrm{AF}}}{4}, \quad E_s = -\frac{3J_{\mathrm{AF}}}{4}.$$

For $h \leq J_{\mathrm{AF}}$, one component of the triplet becomes closer to the singlet ground state such that for a strong enough magnetic field, we have a situation when the singlet and $S^z = 1$ component of the triplet create a different effective spin $\tau = 1/2$ system. On the other singlet-triplet subspace, the original Hamiltonian becomes the Hamiltonian of a fully anisotropic XYZ spin-$\frac{1}{2}$ chain in an effective magnetic field,[14]

$$H_{\mathrm{eff}} = \frac{J_{\mathrm{F}}}{2} \sum_{j=1}^{N/2} \left[-\frac{1}{2} \tau_j^z \tau_{j+1}^z + \Delta \tau_j^y \tau_{j+1}^y + \tau_j^x \tau_{j+1}^x \right] + h^{\mathrm{eff}} \sum_{j=1}^{N/2} \tau_j^z, \tag{2}$$

where $h^{\mathrm{eff}} = h - J_{\mathrm{AF}} + J_{\mathrm{F}}/4$. At $\Delta = 1$, the effective problem reduces to the theory of the XXZ chain with a fixed antiferromagnetic anisotropy of 1/2 in a magnetic field.[2] The gapped Haldane phase at $h^{\mathrm{eff}} < h_{c_1}^{\mathrm{eff}} = -\frac{J_{\mathrm{F}}}{4}$ for the AF-F alternating chain corresponds to the negatively saturated magnetization phase for the effective spin chain, whereas the massless LL phase of the AF-F alternating chain corresponds to the finite magnetization phase of the effective spin-$\frac{1}{2}$ chain. The critical field $h_{c_2}^{\mathrm{eff}} = \frac{J_{\mathrm{F}}}{4}$, where the AF-F alternating chain is totally magnetized, corresponds to the fully magnetized phase of the effective spin chain.

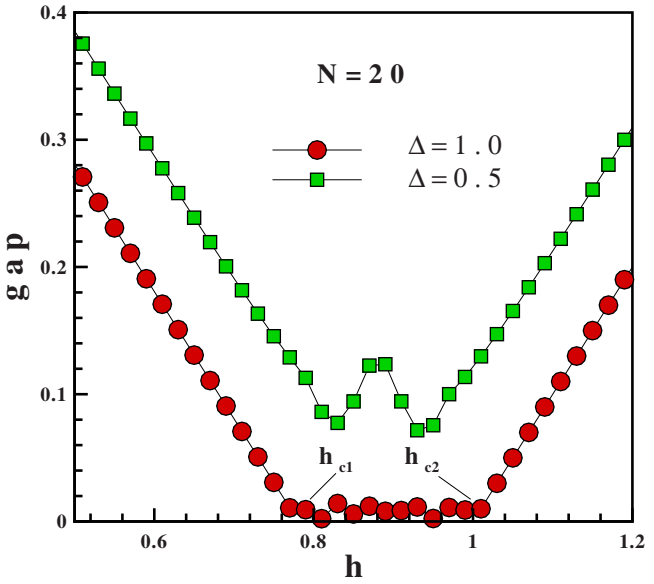

FIG. 1. (Color online) The excitation gap of a spin-$\frac{1}{2}$ AF-F chain versus the uniform magnetic field h for different anisotropy parameters $\Delta = 1.0$ and 0.5 and chain size $N = 20$.

Away from the isotropic point $\Delta = 1$ the effective Hamiltonian (2) describes the fully anisotropic ferromagnetic XYZ chain in a magnetic field that is directed perpendicular to the easy axis. In this case, it is found[14] that a gapped stripe-antiferromagnetic phase exists for the intermediate values of the transverse magnetic field $h_{c_1} < h < h_{c_2}$.

To recognize the different phases induced by the transverse magnetic field in the ground-state phase diagram, we implemented the modified Lanczos algorithm of finite-size chains ($N = 12, 16, 20, 24$) (Ref. 14) with $J_{\mathrm{AF}} = 1$, $J_{\mathrm{F}} = 1/2$ and different values of the anisotropy parameter Δ. The energies of a few lowest eigenstates were obtained for the chains with periodic boundary conditions. In Fig. 1 we have plotted the results of these calculations for different values of the anisotropy parameter $\Delta = 1.0$ and 0.5, and chain length $N = 20$. As it is clearly seen from this figure, in the case of zero magnetic field the spectrum of the model is gapped. For $h \neq 0$ the gap decreases linearly with h and vanishes at the critical field $h_{c_1}(\Delta)$. In the isotropic case $\Delta = 1.0$, the spectrum remains gapless for $h_{c_1} = 0.78 \pm 0.01 < h < h_{c_2} = 1.0$ and becomes once again gapped for $h > h_{c_2}$. But, in the anisotropic case $\Delta = 0.5$, the excitation spectrum is gapful except at two critical-field values $h_{c_1} = 0.82 \pm 0.01$ and $h_{c_2} = 0.94 \pm 0.01$. In the intermediate region $h_{c_1} < h < h_{c_2}$ the spin gap which appears at $h > h_{c_1}$ first increases vs external field and after passing a maximum decreases to vanish at h_{c_2}.

In conclusion, at $T=0$, two quantum phase transitions in the ground-state phase diagram of the model have been identified with increasing transverse magnetic field.[14] The first transition corresponds to the transition from the gapped Haldane phase to the gapless LL phase (or gapped stripe antiferromagnetic for the anisotropic case). The other one is the transition from the gapless LL phase (or gapped stripe antiferromagnetic) to the fully polarized phase.

B. Fermionization

The behavior of the gap and the quantum phase space of the model leads us to investigate the thermodynamic properties of the model. In this respect, we implement the Jordan-Wigner transformation to fermionize the model. Because of the two types of coupling constant, we introduce two kinds of spinless fermion through the following Jordan-Wigner transformations:

$$S_{2n-1}^{+} = a_n^{\dagger} \exp i\pi\left(\sum_{m=1}^{n-1} a_m^{\dagger} a_m + \sum_{m=1}^{n-1} b_m^{\dagger} b_m\right),$$

$$S_{2n}^{+} = b_n^{\dagger} \exp i\pi\left(\sum_{m=1}^{n} a_m^{\dagger} a_m + \sum_{m=1}^{n-1} b_m^{\dagger} b_m\right),$$

$$S_{2n-1}^{z} = a_n^{\dagger} a_n - \frac{1}{2}, \quad S_{2n}^{z} = b_n^{\dagger} b_n - \frac{1}{2}.$$

Using the above transformations, the thermodynamic behavior of the isotropic ($\Delta=1$) Heisenberg AF-F spin-$\frac{1}{2}$ chains has been studied in the absence of a magnetic field.[9] By the above transformations, the AF-F spin chain is mapped onto a 1D system of interacting spinless fermions,

$$\begin{aligned}\hat{H}_f = &-\frac{Nh}{2} + \sum_{n=1}^{N/2}\left(\frac{J_F}{2} - \frac{J_{AF}}{2} + h\right)(a_n^{\dagger} a_n + b_n^{\dagger} b_n) \\ &+ \sum_{n=1}^{N/2}\left(\frac{J_{AF}}{2} a_n^{\dagger} b_n - \frac{1+\Delta}{4} J_F a_{n+1}^{\dagger} b_n \right. \\ &\left. - \frac{1-\Delta}{4} J_F b_n^{\dagger} a_{n+1}^{\dagger} + \text{H.c.}\right) + \sum_{n=1}^{N/2} J_{AF} a_n^{\dagger} a_n b_n^{\dagger} b_n \\ &- \sum_{n=1}^{N/2} J_F b_n^{\dagger} b_n a_{n+1}^{\dagger} a_{n+1}. \end{aligned} \tag{3}$$

Treating the Hamiltonian H_f in the mean-field approximation, the interacting fermionic system reduces to a 1D system of different noninteracting dynamical quasiparticles. Many mean-field order parameters (auxiliary fields) might be considered. Many of them are irrelevant, i.e., they do not have a stable mean-field solution, while some are relevant. In our system we have introduced the magnetization, ferromagnetic, and antiferromagnetic dimers as mean-field order parameters;

$$\langle a_n^{\dagger} a_n \rangle = d_a, \quad \langle b_n^{\dagger} b_n \rangle = d_b,$$

$$\langle a_{n+1}^{\dagger} b_n \rangle = P_F, \quad \langle b_n^{\dagger} a_n \rangle = P_{AF}. \tag{4}$$

Utilizing the above order parameters, the mean-field Hamiltonian is given by

$$\mathcal{H}_{HF} = E_0 + \sum_k \frac{A}{2} a_k^{\dagger} a_k + \frac{B}{2} b_k^{\dagger} b_k + \gamma_k a_k^{\dagger} b_k + \text{H.c.}, \tag{5}$$

where

$$A = (J_{AF} - J_F)(d_b - 1/2) + h,$$

$$B = (J_{AF} - J_F)(d_a - 1/2) + h,$$

$$\gamma_k = J_{AF}(1/2 - P_{AF}) e^{ik/2} + J_F\left(P_F^{*} - \frac{1+\Delta}{4}\right) e^{-ik/2},$$

$$\begin{aligned} E_0 = \frac{N}{2}\Bigg[& J_{AF}(|P_{AF}|^2 - d_a d_b + 1/4) - h \\ & - J_F(|P_F|^2 - d_a d_b + 1/4) - \frac{J_F}{16}(1-\Delta^2)^2 \Bigg]. \end{aligned} \tag{6}$$

In the above equations, $\langle \ldots \rangle$ represents thermal averaging over the Hartree-Fock eigenstates. d_a and d_b are related to the magnetization, and P_F and P_{AF} are ferromagnetic and antiferromagnetic exchange order parameters, respectively. It is clear that $P_{AF}(P_F)$ in the Hilbert space is the AF(F)-dimer order parameter, i.e.,

$$\langle S_{2n}^{-} S_{2n+1}^{+} \rangle = \langle a_{n+1}^{\dagger} b_n \rangle = P_F,$$

$$\langle S_{2n-1}^{-} S_{2n}^{+} \rangle = \langle b_n^{\dagger} a_n \rangle = P_{AF}. \tag{7}$$

Using the following unitary transformations:

$$a_k = u_k \alpha_k + v_k e^{i\theta_k} \beta_k,$$

$$b_k = v_k e^{-i\theta_k} \alpha_k + u_k \beta_k,$$

the diagonalized Hamiltonian is given by

$$\mathcal{H} = E_0 + \sum_k \sum_{\sigma=\pm} (\epsilon_k^{+} \alpha^{\dagger} \alpha_k + \epsilon_k^{-} \beta^{\dagger} \beta_k), \tag{8}$$

$$\epsilon_k^{\pm} = \xi \pm \sqrt{\eta^2 + \gamma_k^2} + h,$$

$$\eta = \frac{B-A}{2}, \quad \xi = \frac{B+A}{2}. \tag{9}$$

Equation (6) clearly shows that the effect of the anisotropy appears in the dispersion relations. The dispersion relations of low-lying excitation read as

$$\epsilon_k^{\pm} \cong \pm [(J_{AF}\tilde{P}_{AF} - J_F\tilde{P}_F)^2 + J_{AF}J_F\tilde{P}_{AF}\tilde{P}_F k^2]^{1/2} + h,$$

where $\tilde{P}_{AF} = 1/2 - \text{Re}\, P_{AF}$ and $\tilde{P}_F = \frac{1+\Delta}{4} - \text{Re}\, P_F$. Using the above order parameters, the thermodynamic functions, such as the internal energy and the specific heat, are expressed as follows:

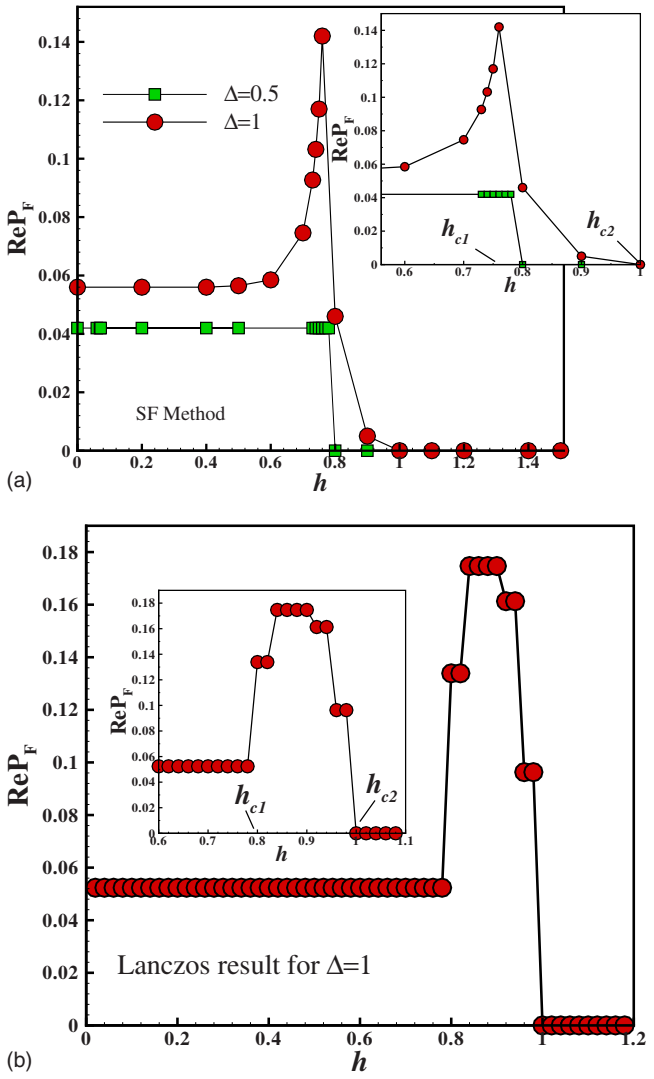

FIG. 2. (Color online) (a) The spinless fermion results of the real part of the ferromagnetic exchange order parameter at temperature $T=0.05$ versus h for $J_{AF}=1$ and $J_F=0.5$. (b) Exact diagonalization Lanczos results of the real part of the P_F for a chain size $N=20$.

$$U = E_0 + \sum_k \sum_{\sigma=\pm} \epsilon_k^\sigma \bar{n}_k^\sigma,$$

$$C = \frac{\partial U}{\partial T}, \tag{10}$$

where $\bar{n}_k^\sigma = [e^{\epsilon_k^\sigma/T}+1]^{-1}$ is the fermion distribution function (choose $k_B=1$).

In order to obtain the thermodynamic behavior of the system, we need to know the whole temperature behavior of the order parameters for different values of h. The order parameters satisfy a set of self-consistent equations and it should be solved the Eq. (4) self-consistently.

In Fig. 2(a), we have plotted the ferromagnetic dimer order parameter of both anisotropic ($\Delta=0.5$) and isotropic ($\Delta=1$) AF-F Heisenberg spin-$\frac{1}{2}$ chains versus h. The curves have been plotted close to the zero temperature. As we mentioned, at $T=0$ for different values of h, our 1D system experiences three phases. In the Haldane phase ($h<h_{c_1}$), the quantum fluctuations are strong enough to suppress the ferromagnetic order of the system and the AF(F)-dimer parameters $P_{AF}(P_F)$ should be close to the classical value $-0.5(0)$.[34] In this region the energy spectrum is gapped and the gap is decreased by increasing h.

The first quantum phase transition occurs at h_{c_1}. At the same time the fermionic band starts to be filled where the excited state sticks to the ground state and the gap of the system is closed. For the first region there is no specific difference between the two anisotropic and isotropic cases, i.e., anisotropy shows a marked behavior for the case of $h_{c_1}<h<h_{c_2}$.

For the case of $\Delta=1$ and $h=0$, the system is isotropic and has SU(2) rotational symmetry. In the intermediate region this system is gapless and correlations decay in a power law.[26] In this region, the Luttinger liquid phase, the magnetic field suppresses quantum fluctuations and induces quasi-long-range order in the 1D system. Although the power-law behavior of the correlations and other properties of the LL phase are manifest, the lack of an order parameter that show the behavior of the system in this phase is still felt. As it is obviously seen in Fig. 2, the F-dimer order parameter has a considerable value in this region and is sensitive to h. The value of this order parameter falls sharply at the second critical field where the fermionic band is completely filled and the gap of the system is reopened.

We have also plotted in Fig. 2(b) the F-dimer order parameter of the isotropic AF-F Heisenberg spin-$\frac{1}{2}$ chain by using the exact diagonalization Lanczos results. The numerical Lanczos method is implemented as a reference approach to see the accuracy of our spinless fermion method. As it is clearly observed in Fig. 2(b) the results of Lanczos method confirm that the defined mean-field order parameter has a considerable value for the intermediate values of field.

We have also plotted in Fig. 2 the F-dimer order parameter of anisotropic F-AF spin-$\frac{1}{2}$ chain versus transverse magnetic field. Regarding the anisotropy in ferromagnetic coupling, the anisotropic system is mapped to a 1D XYZ model with U(1) symmetry. In the intermediate region ($h_{c_1}<h<h_{c_2}$) the system has the magnetic long-range order and spins are aligned stripe antiferromagnetically. This phase is gapful, and the F-dimer order has no considerable value in this phase. Moreover, there is a big discrepancy between the values of the F dimers of the isotropic and anisotropic cases, i.e., in the LL gapless phase the behavior of the F-dimer order parameter (Re P_F) is different from those of the gapped phases. Therefore, we can conclude that the above F-dimer order parameter can distinguish between the gapless LL phase and the other gapped phases.

This means that experimenters might look for such behavior in Re P_F at finite temperatures. That is, experimental results on this quantity may be used to distinguish between the isotropic chains and anisotropic ones (gapped stripe-antiferromagnetic and gapless LL phases).

III. THERMAL BEHAVIOR OF THE MODEL

In this section we will study the thermal behavior of the mean-field order parameters of the Heisenberg spin-$\frac{1}{2}$ AF-F

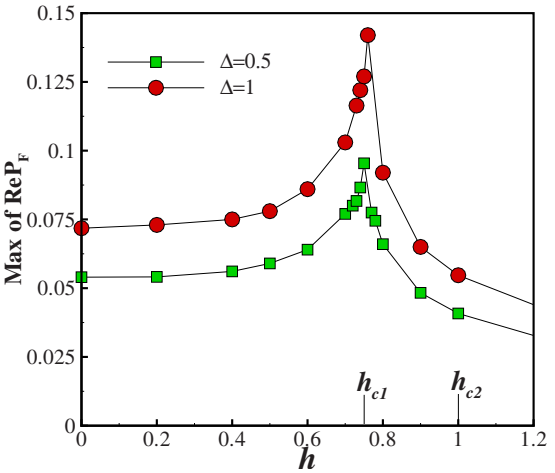

FIG. 3. (Color online) The spinless fermion results of the real part of the ferromagnetic exchange order parameter at temperature T_F versus h for $J_{AF}=1$ and $J_F=0.5$.

chains in both anisotropic and isotropic cases. The order parameters also have different behavior for different values of h.

For $h<h_{c_1}$, in the Haldane phase, an increase in temperature increases the thermal fluctuations and Haldane ordering is suppressed. The solution of Eq. (4) shows that the AF-dimer order parameter (Re P_{AF}) decreases with temperature.

However, J_F couplings supply an interaction between the unit cells and try to establish F-dimer order (Re P_F) even at moderate temperatures (scaled with J_F), i.e., (Re P_F) increases with temperature up to T_F (see Fig. 3). Above T_F, fluctuations are large enough to decrease Re P_F. The locations of the maximum value of (Re P_F) with respect to h are shown in Fig. 3. As it is obviously seen in this plot, there is a peak at h very close to the first critical field. The location of this peak is a good candidate to find the first critical point.

By increasing the magnetic field, the value of T_F (location of the maximum value of Re P_F) decreases. It is found that

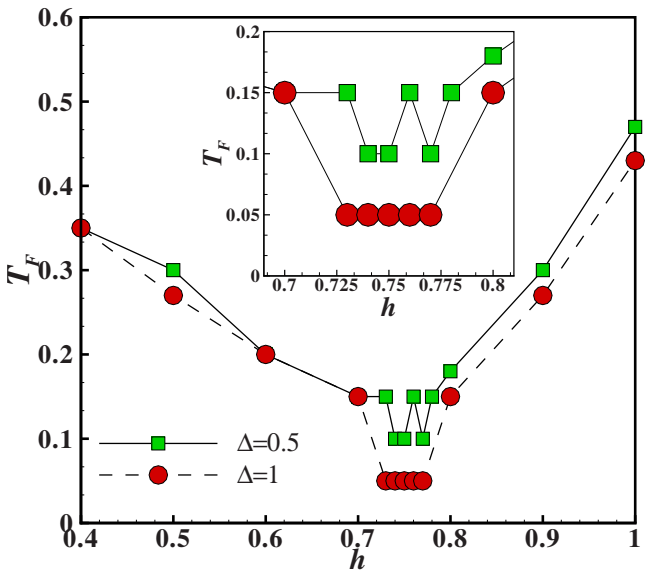

FIG. 4. (Color online) The spinless fermion results for T_F versus h with $J_{AF}=1$ and $J_F=0.5$.

T_F goes to a minimum (Fig. 4) when h increases up to h_{c_1}. Increasing the magnetic field further and for $h_{c_1}\sim 0.76<h<h_{c_2}\sim 1$, T_F always maintains a minimum value and the value of Re P_F decreases monotonically with increasing T. Upon increasing the magnetic field even further, for $h>h_{c_2}$, T_F also increases. The SF calculations also show that the behavior of T_F is similar to the energy gap (see Fig. 1).

The discovery of gapless or gapped excitations has led to the investigation of the thermodynamic properties of the model.[35] One of the most important thermodynamic functions is the specific heat. In this respect, we study the temperature dependence of the specific heat of the model in different quantum regimes. We have calculated the specific heat of both isotropic and anisotropic cases using two methods: the analytical SF and the numerical full diagonalization methods. In Figs. 5(a) and 5(b) we have plotted the results of the SF method in the form of the specific heat C/N versus T with $\Delta=1$ and 0.5 for different values of h. As it is clearly seen in this figure, in the Haldane and paramagnetic regions ($h<h_{c_1}$ and $h>h_{c_2}$, respectively), there is only one peak on

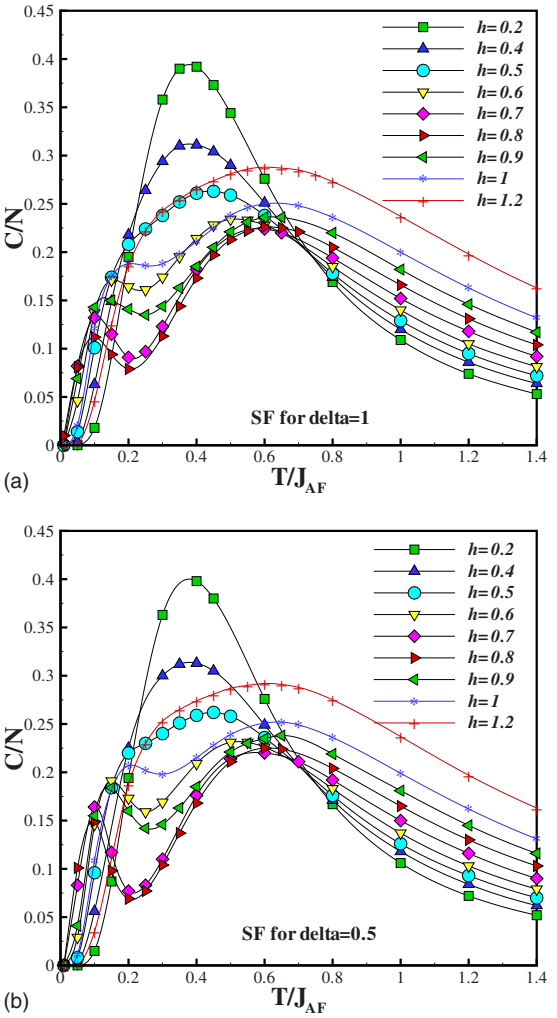

FIG. 5. (Color online) The spinless fermion results of the specific heat of an alternating AF-F spin-$\frac{1}{2}$ chain versus T for different values of the magnetic field h with $J_{AF}=1$ and $J_F=0.5$. (a) $\Delta=1$ and (b) 0.5.

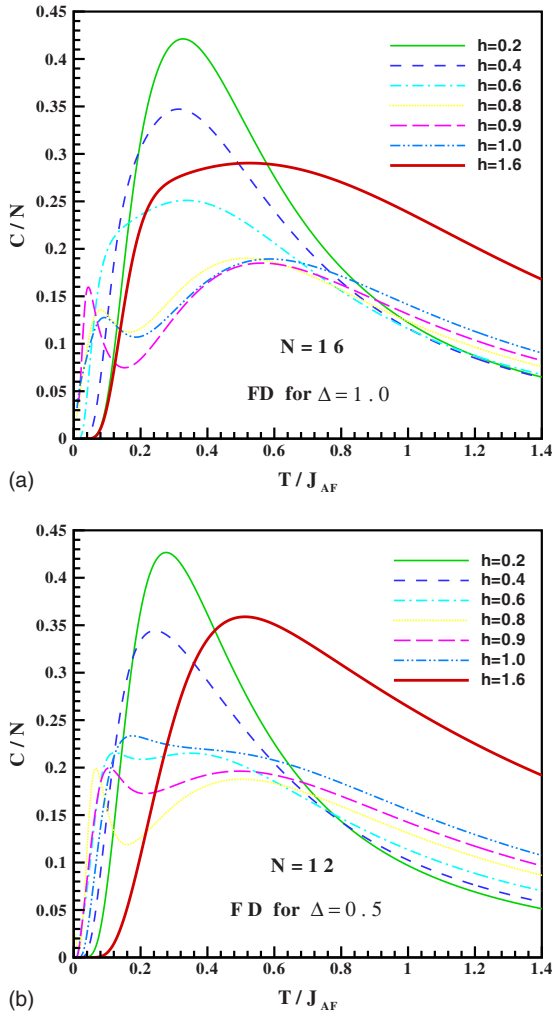

FIG. 6. (Color online) Full diagonalization results of the specific heat of an alternating AF-F spin-$\frac{1}{2}$ chain versus T for different values of the magnetic field h with $J_{\mathrm{AF}}=1$ and $J_{\mathrm{F}}=0.5$. (a) $\Delta=1$ and (b) 0.5.

the specific-heat curve. However, in the intermediate region ($h_{c_1}<h<h_{c_2}$) a double peak is observed. At $h=0$ there is a Schottky-type peak in the specific heat which is expected from the Haldane phase. By increasing h, the peak becomes wider and goes to lower temperatures. Increasing h further causes a shoulder to appear on the right-hand side of the curve. For $h>h_{c_1}$, by increasing h, an additional peak appears which is the signal for the paramagnetic phase. Because of the two F and AF interactions (J_{F} and J_{AF}), there are two kinds of quasiparticles in the system. These quasiparticles have two different dynamics. These dynamics bring about two energy scales in the system. The energy scales affect the behavior of the response functions. It is obviously seen in the plots of the specific heat C/N that the energy scales create a double peak in the specific heat at two different temperatures. As a general statement, two energy scales can produce a double peak structure in the specific heat.

We have also plotted in Figs. 6(a) and 6(b) the specific heat of the model by using the full diagonalization method. We have computed all the eigenvalues of the energies for different values of the transverse magnetic field h and anisotropy parameter Δ. Therefore, using these eigenenergies, we have computed the specific heat as a function of the temperature T. The specific-heat curves have been plotted for $J_{\mathrm{AF}}=1$ and $J_{\mathrm{F}}=0.5$, and for the anisotropy parameters (a) $\Delta=1$ and (b) 0.5. As it is clearly seen in these figures, in the Haldane and paramagnetic regions ($h<h_{c_1}$ and $h>h_{c_2}$, respectively), there is only one peak in the specific-heat curve. To see the qualitative agreement between spinless fermion results and full diagonalization ones, we have plotted the specific heat versus T for an intermediate value of h (for example, $h=0.9$). As it is seen in Fig. 7 the mean-field results are in agreement with the others qualitatively. It is interesting that the numerical results confirm the existence of the double peak in the intermediate region ($h_{c_1}<h<h_{c_2}$).

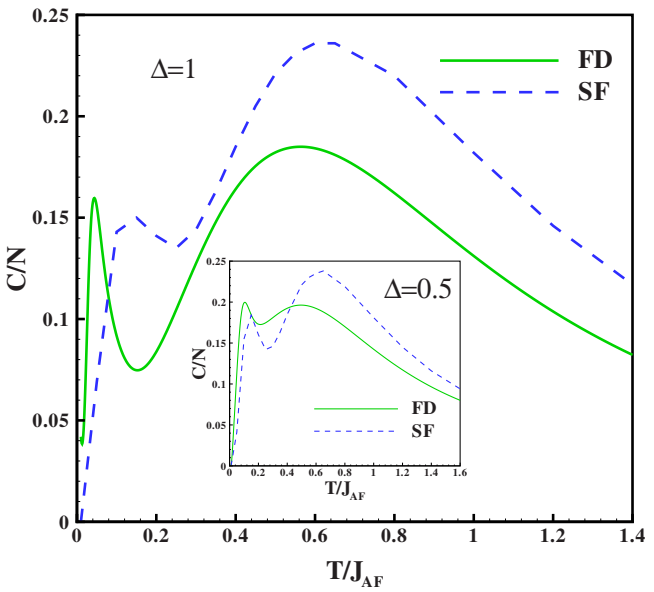

FIG. 7. (Color online) Specific heat of the AF-F Heisenberg spin-$\frac{1}{2}$ chain vs T for both values of Δ and $h=0.9$ using the SF and FD approaches.

IV. CONCLUSION

To summarize, we have studied the zero- and finite-temperature behaviors of the anisotropic alternating AF-F Heisenberg spin-$\frac{1}{2}$ chains in a transverse magnetic field. The numerical exact diagonalization method and analytical spinless fermion approach are applied to analyze the model. The first notable point is introducing a different mean-field order parameter which can distinguish between a gapless LL phase and the gapped phases. This order parameter in the spin language of Hilbert space is the F-dimer order parameter. In the isotropic case, the F-dimer order parameter has a considerable value in the LL region. We have shown that there is a big discrepancy between the values of the F dimers of the isotropic and anisotropic cases, i.e., in the LL gapless phase the behavior of the F-dimer order parameter (Re P_{F}) is different from that of the gapped phases. Therefore, we have concluded that the F-dimer order parameter can distinguish the gapless LL phase from the other gapped phases.

The second notable point is found from the specific heat. We have obtained a double peak structure in the specific-heat curves vs temperature.

There are some questions behind the defined order parameter which are still controversial, and we can investigate them in future. The most remarkable questions referred to the topological order and spontaneous symmetry breaking. That is, in the LL phase, where the real part of the F dimer is not zero, how can one describe topological order and what kind of spontaneous symmetry breaking occurs?

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