Density-matrix renormalization-group study of $S = \frac{1}{2}$ Heisenberg spin chains: Friedel oscillations and marginal system-size effects

Tai-Kai Ng

Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay Road, Kowloon, Hong Kong

Shaojin Qin

International Center for Theoretical Physics, P.O. Box 586, 34100 Trieste, Italy

Zhao-Bin Su

Institute of Theoretical Physics, P.O. Box 2735, Beijing 100080, People's Republic of China

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We report a density-matrix renormalization-group (DMRG) study of $S = 1/2$ antiferromagnetic Heisenberg spin chains. We show the Friedel oscillations in open spin chains within bosonization theory. The bosonization predictions are in excellent agreement with the DMRG calculation. The chain length dependence of the ground state and several low-energy excited state energies are compared with conformal field theory results. Based upon the DMRG calculations for various quantities, the interplay between the system size and the number of optimal states kept in the DMRG is carefully discussed. [S0163-1829(96)05337-4]

I. INTRODUCTION

Due to the discovery of cupric oxide superconductors, there has been revived interest in low-dimensional quantum spin- $\frac{1}{2}$ antiferromagnetism. Particularly, quite a few new synthesized quasi-one-dimensional oxides exhibit strong quantum spin correlations. It has attracted also extensive studies from both the experimental and theoretical sides. It has been shown that impurities break chains up to finite sections with essentially free boundary conditions.¹ Theoretical study² and experiments³ have shown recently special features near momentum π for such system. So it is very interesting to study the staggered responses of a spin- $\frac{1}{2}$ chain to open boundary conditions. The application of the density-matrix renormalization-group (DMRG) method to these doped or undoped quasi-one-dimensional spin systems is not only because it is a powerful method, but also because the spin systems provide reliable means for exploring the method's applicability to different kinds of physical quantities.

The development of the DMRG method initiated by White⁴ opens a possibility that a variety of systems can be solved numerically with extremely high accuracy, with system size much larger than those solved by exact diagonalization. This method has been successfully applied to various one-dimensional or quasi-one-dimensional quantum systems,⁵ such as antiferromagnetic spin chains, Hubbard chains, Kondo insulator, etc. Its application is still blooming. On the other hand, for such a newly proposed powerful numerical method, its convergence problem has not been thoroughly studied yet. For a targeted antiferromagnetic quantum spin-1 chain, White and Huse demonstrated that⁶ the error of the DMRG calculation decreases exponentially (roughly) along with the increasing of the number of optimal states kept.⁷ But the interplay between the system size and the number of optimal states kept has not been investigated.

In this paper, based on a DMRG study for the quantum spin- $\frac{1}{2}$ chain,⁶ we calculate via the DMRG method the

boundary effect on the spin-spin correlation function and the spin density as well as dimerization distributions for a antiferromagnetic spin- $\frac{1}{2}$ open chain, which are interesting quantities for impurity-doped quantum spin systems. Based on previous studies,⁸⁻¹⁰ we expect similar results for doped *half-integer* spin chains. Our results confirm the approximate results obtained from the bosonization method. We applied further the DMRG calculation to the chain length dependence for the ground-state energy and obtain excellent agreement with results derived from the conformal field theory. We therefore show that the DMRG methods are successful in uncovering the low-energy state properties of such a gapless system. As a final interesting result, which is complementary to those of White and Huse,⁶ we find a sort of marginal size for each fixed number of optimal states kept. If the system goes beyond the marginal size, the error will increase exponentially (roughly) with the increasing of system size. Furthermore, if we increase the number of kept optimal states, the marginal size will move upward so that the convergence would be still further improved.

The arrangement of the paper is as follows: In Sec. II we shall give a brief review of bosonization theory of an $S = 1/2$ spin chain under open boundary conditions (OBC's) where predictions of the theory on the spin-spin correlation function, magnetization distribution $\langle S_i^z \rangle$, and spin bond magnitude $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$ will be derived. In particular a strong finite-size effect associated with spin dimerization will be pointed out. The DMRG numerical results on these quantities will be presented in Sec. III, where comparison between bosonization theory and numerical results will be made. In Sec. IV we shall present our results on the length dependence of the ground-state energy and excitation energy spectrum computed in the DMRG method with a different number of optimal states being kept. Corresponding results on spin chains with periodic boundary conditions (PBC's) will also be given. The results will be compared with exact conformal

field theory predictions. Based on the systematic comparison the reliability of the DMRG method will be discussed.

II. BOSONIZATION THEORY OF AN OPEN $S=1/2$ SPIN CHAIN

We consider the $S=1/2$ open Heisenberg spin chain with Hamiltonian

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

where S_i^+ , S_i^- are the usually spin raising and spin lowering operators at site i , and S_i^z is the z component of spin. For PBC the l th and first site are also coupled with the same J and J_z . The above Hamiltonian can be transformed to a problem of spinless fermions via a Jordan-Wigner transformation, resulting in the Hamiltonian^{11,1,12}

$$H = \sum_{i=1}^{l-1} \left[\frac{J}{2} (\psi_i^\dagger \psi_{i+1} + \text{H.c.}) + J_z \left(\psi_i^\dagger \psi_i - \frac{1}{2} \right) \times \left(\psi_{i+1}^\dagger \psi_{i+1} - \frac{1}{2} \right) \right], \quad (2)$$

where ψ_i and $\psi_i^\dagger$ are spinless fermion annihilation and creation operators, respectively. In the low-energy limit, a continuum theory of the above model can be derived by introducing left- and right-moving fermion fields $\psi_L(x)$ and $\psi_R(x)$. For PBC's the left and right fermions are independent entities, whereas for OBC's, they are related to each other with $\psi_L(x) = -\psi_R(-x)$. The resulting Hamiltonian can be expressed in terms of the fermion currents $J_I(x) = :\psi_I^\dagger(x)\psi_I(x):$, where $I=L,R$ are left- and right-moving branches of the one-dimensional fermions, and

$$H_{\text{continuum}} \sim \pi v \int dx [J_R(x)J_R(x) + J_L(x)J_L(x) + 2bJ_L(x)J_R(x)], \quad (3)$$

where $b=2J_z/(\pi J)$ and v is the renormalized fermion (spin-wave) velocity. For a spin chain with PBC's, this model can be transformed into a boson model (Abelian bosonization) with^{11,1,12}

$$J_R = \frac{-1}{\beta} \left(\Pi_\phi - \frac{\partial \phi}{\partial x} \right),$$

$$J_L = \frac{1}{\beta} \left(\Pi_\phi + \frac{\partial \phi}{\partial x} \right), \quad (4)$$

where $\beta=(4\pi)^{1/2}$, ϕ is a real boson field, and Π_ϕ is the momentum variable conjugate to ϕ . The Hamiltonian (3) can be written in terms of the boson variables as

$$H = \frac{v}{2} \left[(1-b)\Pi_\phi^2 + (1+b) \left(\frac{\partial \phi}{\partial x} \right)^2 \right].$$

It is more convenient to write the Hamiltonian in the normalized form by rescaling the boson operators:

$$\phi = \frac{\phi'}{\beta R},$$

$$\Pi_\phi = (\beta R) \Pi_{\phi'}, \quad (5)$$

where

$$H = \frac{v}{2} \left[(\Pi_{\phi'})^2 + \left(\frac{\partial \phi'}{\partial x} \right)^2 \right], \quad (6)$$

and $R^2 \sim (1+b)/4\pi$ is the rescaling parameter in perturbation theory (small b limit). For general J_z , R can be determined from the Bethe ansatz solution. In particular, in the isotropic limit $J_z=J$, $R^2=1/2\pi$ and $v=\pi/2$.

The left and right fermion fields can be written in terms of the boson variables as

$$\psi_R \sim \exp \left(-i2\pi R(\phi'_L - \phi'_R) - \frac{i}{2R}(\phi'_L + \phi'_R) \right),$$

$$\psi_L \sim \exp \left(-i2\pi R(\phi'_L - \phi'_R) + \frac{i}{2R}(\phi'_L + \phi'_R) \right), \quad (7)$$

where

$$\phi' = \phi'_L + \phi'_R,$$

$$\Pi_{\phi'} = \frac{\partial}{\partial x}(\phi'_L - \phi'_R). \quad (8)$$

For OBC's, $\psi_L(x) = -\psi_R(-x)$ and the corresponding ϕ_L and ϕ_R fields are not independent. Using Eq. (4) we obtain $\phi_R(x,t) = \pi - \phi_L(-x,t)$ or, in terms of the normalized variables,¹

$$\phi'_R(x,t) = \pi R - \phi'_L(-x,t),$$

$$\phi'(0) = \pi R,$$

$$\phi'(L) = 2\pi R \left(S^z + \frac{1}{2} \right), \quad (9)$$

where the last two equalities arise from the boundary condition that the original fermion fields should vanish on the zeroth and $(l+1)$ th sites.¹ $S^z = \sum_i S_i^z$ is the z component of total spin, and is integer (half-integer) for chains with an even (odd) number of sites. The boson fields ϕ' and $\Pi_{\phi'}$ can be expanded in terms of normal modes under the boundary conditions (9). We obtain

$$\phi'(x,t) = 2\pi R \left(\frac{1}{2} + S^z \frac{x}{l} \right) + \sum_{n>0} \left(\frac{1}{\pi n} \right)^{1/2} \times \sin(q_n x) [b_n e^{-iq_n t} + b_n^\dagger e^{iq_n t}],$$

$$\Pi'_{\phi'}(x,t) = \frac{-i}{l} \sum_{n>0} (n\pi)^{1/2} \sin(q_n x) [b_n e^{-iq_n t} - b_n^\dagger e^{iq_n t}], \quad (10)$$

where $q_n = n\pi/l$, and b_n and $b_n^\dagger$ are boson annihilation and creation operators, respectively. The resulting energy spectrum is given by

$$H = \frac{\pi v}{l} \left[2\pi R^2 (S^z)^2 + \sum_{n>0} b_n^\dagger b_n \right]. \quad (11)$$

The spin operators can also be written in terms of the boson fields following standard procedures.¹ We obtain

$$S_j^- \sim e^{i2\pi R(\phi_L' - \phi_R')} \left[\text{const} \times \sin \frac{\phi'}{R} + (-1)^j \times \text{const} \right],$$

$$S_j^z \sim \frac{1}{2\pi R} \frac{\partial \phi'}{\partial x} + (-1)^j \times \text{const} \times \sin \frac{\phi'}{R}. \quad (12)$$

We shall also be interested at the spin-Peierls operator $D_i = \mathbf{S}_i \cdot \mathbf{S}_{i+1} - \mathbf{S}_i \cdot \mathbf{S}_{i-1}$ which measures the “staggered” part of the bond amplitude $\mathbf{S}_i \cdot \mathbf{S}_{i+1}$. In terms of the boson fields, D_i can be written as¹

$$D_i \sim \text{const} \times \cos \frac{\phi'}{R}. \quad (13)$$

In the following we shall apply the bosonization formulas to examine several properties of open $S=1/2$ spin chains. First we study the (ground-state) spin-spin correlation function $\langle \mathbf{S}_i(t) \cdot \mathbf{S}_j(t') \rangle$. The staggered part of the spin-spin correlation function can be extracted quite easily using Eq. (12) and Eq. (10). In the continuum limit and in the limit $x, x' \ll l$, we obtain

$$\langle \mathbf{S}(x, t) \cdot \mathbf{S}(x', t') \rangle$$

$$\sim (-1)^{(\Delta x)} \left(\frac{xx'}{[(\Delta x)^2 - (v\Delta t)^2][(x+x')^2 - (v\Delta t)^2]} \right)^{1/2}, \quad (14)$$

where $\Delta x = x - x'$ and $\Delta t = t - t'$, in exact agreement with previous result obtained by Eggert and Affleck.¹ Notice that away from the boundary, when $xx' \gg |(\Delta x)^2 - (v\Delta t)^2|$, the usual bulk correlation function is recovered, whereas the correlation function near the boundary is modified strongly by the boundary effect.

We shall also examine the magnetization distribution $\langle S_i^z \rangle$ and dimerization (spin-Peierls) distribution $\langle D_i \rangle$ for lowest-energy states with fixed total z component of spin S^z 's. The ground state corresponds to the lowest-energy state with $S^z = 0$. For states with $S^z \neq 0$, the magnetization $\langle S_i^z \rangle$ will be distributed unevenly in the spin chain because of OBC's. The staggered part of the magnetization distribution $\langle S_i^z \rangle$ can again be computed easily in the continuum limit using Eq. (12) and Eq. (10). We obtain for $x \ll l$, $\langle S^z(x) \rangle = \langle m(x) \rangle + (-1)^x \langle n(x) \rangle$, where

$$\langle n(x) \rangle \sim \sin \left(\frac{2\pi S^z x}{l} \right) \left(\frac{a^2}{a^2 + x^2} \right)^{1/4}, \quad (15)$$

where a is a constant $\sim$ lattice spacing.

The spin-Peierls distribution $\langle D_i \rangle$ can be computed similarly using Eq. (13) and Eq. (10). We obtain

$$\langle D(x) \rangle \sim \cos \left(\frac{2\pi S^z x}{l} \right) \left(\frac{a^2}{a^2 + x^2} \right)^{1/4}. \quad (16)$$

Notice that for chains with PBC's, both $\langle n(x) \rangle$ and $\langle D(x) \rangle$ should be zero because of translational invariance. For open spin chains $\langle n(x) \rangle$ and $\langle D(x) \rangle$ are expected to be sizable only at the boundary, and should decay to zero away from the boundary. Bosonization theory predicts that the decay rate is extremely slow [$\sim (1/x)^{1/2}$] for both $\langle n(x) \rangle$ and $\langle D(x) \rangle$. The oscillatory factors $\sin(\cos)(2\pi S^z x/l)$ can be understood easily by the mapping of the Heisenberg model to spinless fermions model [Eq. (2)]. The number of spinless fermions in the system is $l/2 + S^z$ with a corresponding “Fermi wave vector” $k_F = (l/2 + S^z)\pi/l$. The “Fermi surface” of the spinless fermions gives rise to Friedel-type oscillations

$$\sim e^{i2k_F x} \sim (-1)^x \exp \left(i \frac{2\pi S^z}{l} x \right),$$

leading to the observed oscillatory behavior in the staggered functions $\langle n(x) \rangle$ and $\langle D(x) \rangle$. Notice that the slow decay rate of the ground-state dimerization amplitude $\langle D(x) \rangle \sim (1/x)^{1/2}$ is expected to be an universal behavior for *half-integer* spin chains and is absent in integer spin chains where $\langle D(x) \rangle \sim e^{-x/\xi}$, where ξ is the correlation length.^{8,9}

In the next section we shall present results of the DMRG calculation for an $S=1/2$ spin chain with 100 sites where the numerical results will be compared with bosonization predictions in this section. We shall see that the numerical DMRG results are in good qualitative agreements with predictions based on the bosonization technique.

III. DMRG RESULTS FOR AN $S=1/2$ SPIN CHAIN

A previous DMRG study has proved to be tremendously successful in computing ground-state energies of $S=1/2$ antiferromagnetic Heisenberg spin chains.⁴ In this section we apply the method to study several ground-state and excited-state properties of an open $S=1/2$ spin chain where the results will be compared with bosonization predictions discussed in the previous section. We use the infinite chain algorithm⁴ in our study. Two new sites are added to the spin chain in each optimal step of the calculation from length $L=4$ to $L=100$. That is, open spin chains with an *even* number of sites are studied. The number of the kept optimized states in our calculation is $m=120$. The largest truncation error is found to be smaller than 10^{-10} when the chain length reaches $L=100$ in the final step. Properties of the ground state and a few lowest excited states are obtained by looking at the *lowest*-energy state obtained in the DMRG method for fixed given total z component of spin $S^z = \sum_i S_i^z$. We shall look at the excitation energies of various states with different S^z and shall study the corresponding average z component of spin on each site $i = \langle S_i^z \rangle$ and dimerization parameter $D(i) = \langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} - \mathbf{S}_i \cdot \mathbf{S}_{i-1} \rangle$.

In Fig. 1 we present the excitation energies $E_n - E_0$ for $n=1-3$ as a function of inverse chain length l^{-1} for the spin chain. E_n is the energy of the lowest state obtained in the DMRG calculation in the sector $S^z = n$. Energy is measured in units of the Heisenberg coupling J . According to the bosonization prediction [Eq. (11)], the excitation energy is given by

FIG. 1. The excitation energy $E_n - E_0$ for an even $S = 1/2$ open chain as a function of inverse chain length $1/l$. The lines are bosonization results $E_n - E_0 = n^2 v \pi / l$ with $v = \pi/2$.

$$E_n - E_0 = (S^z)^2 \left(\frac{\pi v}{l} \right),$$

where $\langle b_n^\dagger b_n \rangle = 0$ for the lowest-energy state. The bosonization prediction is also shown in Fig. 1 (dashed lines). Notice that bosonization theory is correct only at the limit $l \rightarrow \infty$ and terms of order $[l \ln(l)]^{-1}$ are neglected. A more careful examination of the DMRG energy spectrum will be given in the next section where our numerical results will be compared with conformal field theory predictions.

Next we consider the equal-time ground-state spin-spin correlation function $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$. At distances $x, x' \ll l$ and $|x - x'| \gg 1$, the staggered part of the spin-spin correlation function is given by Eq. (14), with $\Delta t = 0$. In Fig. 2 we plot the product function $\langle S_i^z S_j^z \rangle |x_i - x_j|$ as a function of x_j for fixed $x_i = 5$ (fifth site from end of spin chain). The (top)

FIG. 2. The ground-state spin-spin correlation $\langle S_i^z S_j^z \rangle$ for an even $S = 1/2$ open chain with $i = 5$. We plot $|i - j| \langle S_i^z S_j^z \rangle$ vs j in the figure. The bottom line is the bosonization prediction for chains with periodic boundary conditions, $|i - j| \langle S_i^z S_j^z \rangle \sim \text{const}$, and top line is the corresponding prediction for open boundary conditions, $|i - j| \langle S_i^z S_j^z \rangle \sim [ij/(i+j)^2]^{1/2}$.

FIG. 3. The ground-state spin-spin correlation $\langle S_i^z S_j^z \rangle$ for an even $S = 1/2$ open chain with $i = 20$. We plot $|i - j| \langle S_i^z S_j^z \rangle$ vs j and the lines have same meaning as in Fig. 2.

dotted line is the spin-spin correlation function given by Eq. (14) and the (bottom) dashed line is the usual spin-spin correlation function for periodic system ($\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle \sim 1/|x_i - x_j|$). In Fig. 3 we plot the same functions with a different $x_i = 20$. It is clear from the figures that our numerical results agree qualitatively with the bosonization formula and the boundary effect gets weaker as x, x' move away from boundary.

The magnetization distribution $\langle S_i^z \rangle$ as a function of position i for lowest-energy states with fixed $S^z = 1, 2, 3$ is given in Fig. 4. It is clear that the observed oscillatory behavior in staggered magnetization is in excellent agreement with the bosonization prediction [Eq. (15)]. The same plot with the $S^z = 0$ (ground state) gives $\langle S_i^z \rangle = 0$ for all sites i , also in agreement with bosonization result.

In Fig. 5 we show the bond amplitude $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$ as function of position i for lowest-energy states with fixed $S^z = 0, 1, 2, 3$. It is again clear that the observed oscillatory

FIG. 4. The magnetization distribution $\langle S_i^z \rangle$ as function of position i for lowest-energy states with fixed S^z for an open $S = 1/2$ even chain. The zero lines for $S^z = 1, 2, 3$ are shifted to 1, 2, 3.

FIG. 5. The bond amplitude $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$ as a function of position i for lowest-energy states with fixed S^z for an open $S=1/2$ even chain. The zero lines for $S^z=1,2,3$ are shifted to 1,2,3. The reference lines are site energies for an infinite $S=1/2$ chain, $e_0 = 1/4 - \ln 2$.

behavior in bond dimerization $D(x)$ is in excellent agreement with the bosonization prediction [Eq. (16)] except for the slight discrepancy at the end points for the $S^z=3$ state. We have also examined the chain length dependence of the midpoint dimerization magnitude $D(l/2)$ as a function of chain length l for these $S^z=0-3$ states, and find that $D(l/2) \sim (1/l)^{0.6}$ in our DMRG result, whereas $D(l/2) \sim (1/l)^{0.5}$ in bosonization theory. As pointed out previously, bosonization theory is correct only at the asymptotic $l \rightarrow \infty$ limit; thus the agreement between bosonization and DMRG numerical results is quantitatively fair.

Summarizing, in this section we have presented our DMRG calculation results for several ground- and excited-state properties of an $S=1/2$ spin chain, and find that our results obtained are in qualitative agreement with predictions of bosonization theory. Notice that the DMRG calculations have produced successfully the properties of the low-lying states for the studied gapless system. In the next section, a more quantitative test of the DMRG technique will be given, where the validity of the DMRG technique will be examined more carefully.

IV. COMPARISON OF DMRG RESULTS WITH CONFORMAL FIELD THEORY PREDICTIONS

In this section we try to make a more critical examination of the DMRG method by comparing the DMRG numerical result of eigenstates energies with exact results obtained in conformal field theory^{12,13} where lowest-order logarithmic corrections to bosonization theory predictions are included. We shall compare the chain length dependences of the energies of the ground state and several excited states for DMRG calculations with several different numbers of optimal states kept. We hope that the comparisons will give us insight into the relation between the reliability of the DMRG calculation, the convergence of numerical results for different chain lengths as well as different numbers of optimized states m kept, and truncation errors in the calculation. By comparing

FIG. 6. The excitation energies $E_n - E_0$ for an even $S=1/2$ open chain for $n=1,2,3$. We plot $(E_n - E_0)l$ vs $1/\ln(l)$. Results with three different numbers of optimal states kept are shown in figure ($m=60, 80, 120$). The lines are conformal field theory predictions $(E_n - E_0)l = n^2 v \pi [1 - 1/2 \ln(l)]$ with $v = \pi/2$.

energies of both ground and excited states, we also obtain more information on the validity of the method in application to excited states.

For an $S=1/2$ spin chain with PBC's, the chain length dependence of the ground-state energy is, to order $O(1/l[\ln(l)]^3)$,¹³

$$E_0(l) = e_0 l - \frac{v\pi}{6l} \left[1 + \frac{3}{8[\ln(l)]^3} \right], \quad (17)$$

where $e_0 = 1/4 - \ln 2$ and the energy is measured in units of J . The energies for lowest-energy states with given $S^z = n$ are, to order $O(1/l[\ln(l)]^3)$,¹³

$$E_n - E_0 = \frac{\pi v}{l} (S^z)^2 \left[1 - \frac{1}{2 \ln(l)} \right]. \quad (18)$$

For open spin chains with an even number of sites, a boundary operator $= \mathbf{S}_l \cdot \mathbf{S}_{l+1} \sim (\partial \phi'_L / \partial x)^2$ exists, giving rise to further energy corrections $\sim (1/l)^2$.¹ The corrections are much smaller than the logarithmic corrections discussed above. Thus, to the order of accuracy examined here, spin chains with OBC's and PBC's have the identical excited-state energy expression (18).

In Fig. 6 we plot $l(E_n - E_0)$ as function of $1/\ln(l)$ for $n=1-3$ for open spin chains with an even number of sites up to chain length 100. Data for calculations with different numbers of optimal states m kept are shown in the figure ($m=60, 80$, and 120). It is clear from the figure that as m increased to $m=120$, numerical results at a chain length $l=100$ for $n=1$ and 2 states have already converged rather well to their final point, but the data for $n=3$ state have not yet. Correspondingly, the deviation of DMRG results from the conformal theory predictions increases with increasing n . Here we observe again the important property of the errors in the DMRG calculation:^{4,7} The real error of the final result is roughly exponentially decreasing with increasing number m of the optimized states kept and convergence of numerical results obtained from different m generally implies that the

TABLE I. The truncation errors at the step where chain length is 100. For comparison of different numbers m of optimal states kept and different boundary conditions (BC's).

BC's	m	$S^z=0$	$S^z=1$	$S^z=2$	$S^z=3$
OBC's	60	6×10^{-9}	5×10^{-9}	3×10^{-9}	3×10^{-9}
OBC's	80	9×10^{-10}	6×10^{-10}	4×10^{-10}	3×10^{-10}
OBC's	120	6×10^{-11}	5×10^{-11}	5×10^{-11}	4×10^{-11}
PBC's	120	3×10^{-6}	3×10^{-6}	2×10^{-6}	2×10^{-6}

numerical results are reliable. However, the limitation of the exponential rule has to be emphasized. We observed in our calculation that for fixed m , the error seems to also increase exponentially with length l of the spin chain, and also increase very rapidly with $n \sim$ excitation energy of the state (see Fig. 6).

In a DMRG calculation, it is thus very important to examine the convergence behavior of the numerical results very carefully. Good convergence of numerical results with a given m at a fixed length l for ground-state energy does not necessarily imply that the numerical results are as reliable when applied to study the chain of double length or for excited states. As can be estimated from the figure, for the $n=3$ state, the error in $E_3 - E_0$ is about a few percent of the correct value in our calculations, though the corresponding error for the $n=1$ state can be hardly seen. The rapid increases of error as function of n indicate that although the DMRG method is very good for studying low-energy states of quantum spin chains, it may not be as reliable a tool to study highly excited states or finite-temperature properties of quantum spin systems.

Next we examine the truncation error in the DMRG method. It is commonly accepted that the real error of the DMRG results is larger than the corresponding truncation error. However, the relation between the real error and truncation error is not clear. For open spin 1/2 chains, the largest truncation error is always the one for the last step (and here is the one for length $l=100$). We have listed the largest truncation error for different numbers m of kept optimal states in Table I. Compared with the order of the real errors observed in Fig. 6, we do not find any clear relationship between the two except that the truncation errors are several orders smaller and the real errors decrease as the truncation errors decrease. In particular, we observe that although the truncation errors for different S^z states are similar for a given m , the real errors observed in the DMRG method are very different.

We have also applied the DMRG method to study ground-state energies of spin chains of different lengths in periodic boundary conditions (PBC's). For PBC's, we apply the infinite chain algorithm on the following configuration of the chain:

The asterisks represent the two new sites inserted. The two "Blocks" represented by the two boxes are identical. The

FIG. 7. The ground-state energy E_0 for a periodic spin 1/2 chain up to length 50. The number of kept optimal states is $m=200$. We plot $(E_0 - e_0)l$ vs $1/\ln^3(l)$ with average on-site energy $e_0 = 1/4 - \ln 2$. The line is the conformal field theory prediction $(E_0 - e_0)l = (-v\pi/6)[1 + 3/8\ln^3(l)]$ with $v = \pi/2$.

lines indicate the bonds between the added sites and the blocks. In each step of the DMRG iteration, we optimize the upper half chain or the lower half chain (in the above configuration) into a larger "Block" for the next step. The upper half or the lower half is optimized alternatively. In this way we insert new sites to the right side or to the left side of the "Block" alternatively.

In Fig. 7 we plot $(E_0 - e_0)l$ versus $1/\ln^3(l)$ for PBC chains up to length 50 and number of kept optimal states $m=200$. The excellent agreement between the DMRG result and the asymptotic behavior predicted from conformal field theory [Eq. (17)] is clear. However, if we extend our calculation to longer chain lengths without improving m , we find that the discrepancy between numerical results and theory

FIG. 8. The ground-state energy E_0 for a periodic spin 1/2 chain. Results with three different numbers of optimal states kept are shown in figure ($m=100, 120, 200$). We plot $(E_0 - e_0)l$ vs $1/\ln^3(l)$ with average on-site energy $e_0 = 1/4 - \ln 2$. The line is the conformal field theory prediction $(E_0 - e_0)l = (-v\pi/6)[1 + 3/8\ln^3(l)]$ with $v = \pi/2$.

FIG. 9. The excitation energies $E_n - E_0$ for an even $S = 1/2$ open chain and periodic chain for $n = 1, 2, 3$. The number of kept optimal states is $m = 120$ in both cases. We plot $(E_n - E_0)l$ vs $1/\ln(l)$. The lines are conformal field theory predictions $(E_n - E_0)l = n^2 v \pi [1 - 1/2 \ln(l)]$ with $v = \pi/2$.

diverges exponentially as l increases further (see Fig. 8). In Fig. 8, for a specific length, we see that the DMRG converges as we increase the number of optimal states kept. In the same figure, for a specific number of optimal states kept, we see also a sort marginal size—beyond which the error of the DMRG results increases rapidly. The marginal size increases as we increase the number of the optimal states kept. We point out here that such a DMRG error behavior is a general behavior observed in our studying of the low-lying states for other systems, both gaped or gapless.

In order to compare errors of the DMRG method between different boundary conditions, we also perform a calculation with same number of optimal states $m = 120$ kept for both PBC and OBC cases and their truncation errors are listed in Table I. The PBC case has clearly a larger truncation error. The corresponding $(E_n - E_0)l$ vs $1/\ln(l)$ curves for PBC's and OBC's is plotted in Fig. 9 for comparison. It is also clear that the real error in the PBC calculation is larger than the corresponding OBC case as is commonly accepted. Noted that the PBC data at chain length $l = 100$ for $n = 2$ and 3 have not converged to their final points yet at $m = 120$.

V. SUMMARY

Summarizing, in this paper we have carried out a detailed study of low-energy properties of an $S = 1/2$ antiferromagnetic spin chain using the DMRG method. We have uncovered the Friedel oscillation for open $S = 1/2$ spin chains. We have studied the spin-spin correlation function, magnetization distribution $\langle S_i^z \rangle$, and spin bond magnitude $\langle S_i \cdot S_{i+1} \rangle$ and have shown the excellent agreement between the bosonization prediction and the DMRG calculation. The staggered response of the magnetization distribution and the spin bond magnitude to the boundary is directly shown. By the systematic calculation on $S = 1/2$ chains, we have demonstrated the success of the DMRG method in studying the low-lying energy states for a gapless system.

We have also compared carefully the DMRG numerical results and conformal field theory results. The agreement between theories and numerical results is excellent in the regime where the DMRG results show good convergence as a function of number of optimal states kept m . We have observed that the real errors decrease exponentially with the number of kept optimal states. We point out that the real errors also increase exponentially with chain length and increase very rapidly with excited states energy or S^z . An error of about 10^{-3} is observed, for example, in our DMRG results for the energy of the $S^z = 3$ state. The rapid increase of error as the chain length increases is perhaps not surprising because of cumulative errors in each step of the DMRG iteration. It is more surprising that the error also increases rapidly with increasing energy or S^z and especially that there are no significant changes in the truncation error between states with different S^z . We have so far no good explanation for this behavior.

As demonstrated in our paper, the DMRG method is extremely powerful in the regime when numerical results converge as a function of m . However, for a specific number of optimal states kept, there is a sort of marginal system size. The reliability of the results decreases very rapidly as we move out of the marginal size.

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¹S. Eggert and I. Affleck, Phys. Rev. B **46**, 10 866 (1992).

²S. Eggert and I. Affleck, Phys. Rev. Lett. **75**, 943 (1995).

³M. Takigawa, N. Motoyama, H. Eisake, and S. Uchida, Bull. Am. Phys. Soc. **41**, 230 (1996); D. C. Dender, D. H. Reich, and C. Broholm, *ibid.* **41**, 228 (1996).

⁴S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); Phys. Rev. B **48**, 10 345 (1993).

⁵Clare C. Yu and S. R. White, Phys. Rev. Lett. **70**, 3866 (1993); H. Pang, S. Liang, and J. Annett, *ibid.* **71**, 4377 (1993); R. M. Noack, S. R. White, and D. J. Scalapino, *ibid.* **73**, 882 (1994); S. Qin, S. Liang, Z.-B. Su, and Lu Yu, Phys. Rev. B **52**, 5475 (1995); S. Moukouri and L. G. Caron, *ibid.* **52**, 15 723 (1995); S. Moukouri, L. Chen, and L. G. Caron, *ibid.* **53**, 488 (1996); L. Chen and S. Moukouri, *ibid.* **53**, 1866 (1996); E. S. Sorensen

and I. Affleck, Phys. Rev. Lett. **71**, 1633 (1993); S. R. White, R. M. Noack, and D. J. Scalapino, *ibid.* **73**, 886 (1994); R. Bursill, T. Xiang, and G. A. Gehring, J. Phys. A **28**, 2109 (1995); E. S. Sorensen and I. Affleck, Phys. Rev. B **51**, 16 115 (1995); K. A. Hallberg, P. Horsch, and G. Martinez, *ibid.* **52**, 719 (1995); K. A. Hallberg, *ibid.* **52**, 9827 (1995); F. Fath, Z. Domanski, and R. Lemanski, *ibid.* **52**, 13 910 (1995); W. Wang, S. Qin, Z. Y. Lu, Lu Yu, and Z.-B. Su, *ibid.* **53**, 40 (1996); U. Schollwock and D. Y. K. Ko, *ibid.* **53**, 240 (1996); X. Wang and S. Mallwitz, *ibid.* **53**, 492 (1996); U. Schollwock, Th. Jolicœur, and T. Garel, *ibid.* **53**, 3304 (1996); Y. Nishiyama, K. Totsuka, N. Hatano, and M. Suzuki, J. Phys. Soc. Jpn. **64**, 414 (1995); U. Schollwock and Th. Jolicœur, Europhys. Lett. **30**, 449 (1995).

⁶S. R. White and D. A. Huse, Phys. Rev. B **48**, 3844 (1993).

- ⁷S. Liang and H. Pang, Phys. Rev. B **49**, 9214 (1994).
- ⁸T. K. Ng, Phys. Rev. B **50**, 555 (1994).
- ⁹S. Qin, T. K. Ng, and Z-B. Su, Phys. Rev. B **52**, 12 844 (1995).
- ¹⁰A. Moreo, K. Hallberg, and P. Horsch, Bull. Am. Phys. Soc. **41**, 279 (1996).
- ¹¹See, for example, E. Fradkin, in *Field Theories of Condensed Matter Systems*, edited by E. Fradkin (Addison-Wesley, Redwood City, 1991), for a brief review.
- ¹²See I. Affleck, in *Field Theory Methods and Quantum Critical Phenomena*, edited by E. Brezin and J. Zinn-Justin (North-Holland, Amsterdam, 1990), for a review.
- ¹³I. Affleck, D. Gepner, H. J. Schulz, and T. Ziman, J. Phys. A **22**, 511 (1989).