

## Transfer-matrix density-matrix renormalization-group theory for thermodynamics of one-dimensional quantum systems

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(Received 19 March 1997)

The transfer-matrix density-matrix renormalization-group method for one-dimensional quantum lattice systems has been developed by considering the symmetry property of the transfer matrix and introducing the asymmetric reduced density matrix. We have evaluated a number of thermodynamic quantities of the anisotropic spin-1/2 Heisenberg model using this method and found that the results agree very accurately with the exact ones. The relative errors for the spin susceptibility are less than  $10^{-3}$  down to  $T=0.01J$  with 80 states kept. [S0163-1829(97)02034-1]

The density-matrix renormalization group (DMRG)<sup>1</sup> is a powerful numerical method for studying the ground and low-lying state properties of low-dimensional lattice models. It has been applied successfully to a number of strongly correlated systems at zero temperature in one dimension (1D)<sup>2-6</sup> as well as two dimensions (2D).<sup>7-9</sup> In 1995, Nishino pointed out that as the partition function of a 2D classical system is determined only by the maximum eigenvalue of a transfer matrix in the thermodynamic limit, the DMRG idea can be extended to find this extreme eigenvalue and the corresponding eigenstate. Subsequently one can study thermodynamic properties. He calculated the specific heat of the 2D Ising model using this so-called transfer-matrix DMRG method and found that the result agrees very accurately with the exact solution.<sup>10</sup> Recently, Bursill, Xiang, and Gehring have developed a transfer-matrix DMRG algorithm for 1D quantum systems.<sup>11</sup> They tested the method on the dimerized spin-1/2 XY model and obtained encouraging results. However, a proper implementation of the transfer-matrix DMRG for studying the thermodynamic properties of 1D quantum systems, especially at low temperature, remains challenging.

In this paper, we report our recent progress on the development of the transfer-matrix DMRG method for 1D quantum systems. We have considered the symmetry properties of the quantum transfer matrix<sup>12,13</sup> and introduced an asymmetric reduced density matrix which optimizes truncated basis states. This study allows us to achieve significantly accurate results at low temperature and greatly enhances the applicability of the method. For the  $S=1/2$  Heisenberg antiferromagnetic chain, we found that the relative error for the spin susceptibility is of the order of  $10^{-4}$  down to the temperature  $T=0.01J$  ( $J$  is the exchange constant) with 80 states kept. This size of error and the value of the temperature are smaller than those for typical quantum Monte Carlo results as well as the thermodynamic DMRG results.<sup>14</sup> The thermodynamic DMRG method<sup>14</sup> cannot treat accurately a physical system where the correlated length diverges (for example the low-temperature region of the  $S=1/2$  Heisenberg model) because of the finite-size effect. However, there is no such problem in the transfer-matrix DMRG method

since this method deals directly with an infinite lattice system.

We demonstrate our method using the 1D anisotropic spin-1/2 Heisenberg antiferromagnetic model

$$\hat{H} = \sum_i^N \hat{h}_i; \quad \hat{h}_i = J[\hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y + \Delta \hat{S}_i^z \hat{S}_{i+1}^z]. \quad (1)$$

We shall set  $J=1$ . To apply the DMRG idea, we use the Trotter formula to decompose the partition function.  $\hat{H}$  is separated into two parts,  $\hat{H}_o$  and  $\hat{H}_e$ , containing those terms with  $i$  being odd or even, respectively. The partition function is represented in terms of the quantum transfer matrix  $\mathcal{T}_M$ .<sup>12,13</sup>

$$Z = \lim_{\epsilon \rightarrow 0} \text{Tr}[e^{-\epsilon \hat{H}} e^{-\epsilon \hat{H}_e}]^M = \lim_{\epsilon \rightarrow 0} \text{Tr} \mathcal{T}_M^{N/2}, \quad (2)$$

where  $\epsilon = \beta/M$ ,  $\beta = 1/T$ , and  $M$  is the Trotter number. The elements of the asymmetric matrix  $\mathcal{T}_M$  are determined by the product of  $2M$  local transfer matrices

$$\begin{aligned} & \langle \sigma_1^3 \cdots \sigma_{2M}^3 | \mathcal{T}_M | \sigma_1^1 \cdots \sigma_{2M}^1 \rangle \\ &= \sum_{\{\sigma_k^2\}} \prod_{k=1}^M \tau(\sigma_{2k-1}^3 \sigma_{2k}^3 | \sigma_{2k-1}^2 \sigma_{2k}^2) \\ & \quad \times \tau(\sigma_{2k}^2 \sigma_{2k+1}^2 | \sigma_{2k}^1 \sigma_{2k+1}^1), \end{aligned} \quad (3)$$

with  $\tau(\sigma_{2M}^2 \sigma_{2M+1}^2 | \sigma_{2M}^1 \sigma_{2M+1}^1) = \tau(\sigma_{2M}^2 \sigma_1^2 | \sigma_{2M}^1 \sigma_1^1)$ , imposing periodic boundary conditions in the Trotter direction. The local transfer matrix is given by  $\tau(\sigma_k^{i+1} \sigma_{k+1}^{i+1} | \sigma_k^i \sigma_{k+1}^i) = \langle s_{k+1}^{i+1}, s_{k+1}^i | \exp(-\epsilon \hat{h}_i) | s_k^i, s_k^{i+1} \rangle$  where  $\sigma_k^i = (-1)^{i+k} s_k^i$  and  $|s_k^i\rangle$  is an eigenstate of  $\hat{S}_k^z$ :  $\hat{S}_k^z |s_k^i\rangle = s_k^i |s_k^i\rangle$ . The basis  $|\sigma_k^i\rangle \otimes |\sigma_{k+1}^i\rangle$  is used to represent  $\tau$  and to construct the corresponding Trotter space. The superscripts and subscripts in  $\mathcal{T}_M$  and  $\tau$  represent the coordinates of spins in the real and Trotter space, respectively.

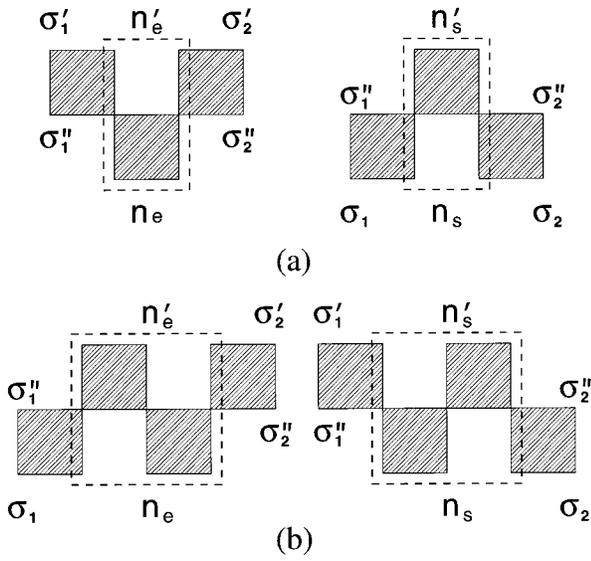


FIG. 1. Configurations of the superblocks: (a)  $M = \text{odd}$  and (b)  $M = \text{even}$ . The left and right transfer matrices are connected, via the summation over states  $\sigma_1''$  and  $\sigma_2''$ , to form a periodic time-slice chain for  $\mathcal{T}_M$ .

The local Hamiltonian  $\hat{h}_i$  conserves the total spin at sites  $i$  and  $i+1$ , i.e.,  $s_k^i + s_k^{i+1} = s_{k+1}^i + s_{k+1}^{i+1}$ . In the Trotter space this conservation law can be expressed as  $\sigma_k^i + \sigma_{k+1}^i = \sigma_k^{i+1} + \sigma_{k+1}^{i+1}$ . This means that  $\tau(\sigma_k^{i+1} \sigma_{k+1}^{i+1} | \sigma_k^i \sigma_{k+1}^i)$  is block diagonal for each value of  $\sigma_k^i + \sigma_{k+1}^i$ . It turns out that the total sum of  $\sigma_k^i$  at site  $i$  is conserved in  $\mathcal{T}_M$ , i.e.,  $\sum_k \sigma_k^i = \sum_k \sigma_k^{i+1}$ , and  $\mathcal{T}_M$  is block diagonal according to the value of  $\sum_k \sigma_k^i$ . For Eq. (1), it can be further proved that the maximum eigenvalue of  $\mathcal{T}_M$  occurs in the  $\sum_k \sigma_k^i = 0$  sub-block.<sup>15</sup> Therefore only the  $\sum_k \sigma_k^i = 0$  sub-block in  $\mathcal{T}_M$  is considered in our DMRG iterations. This consideration allows us to keep more basis states in the truncation of the basis set and to save computer CPU time.

In the limit  $N \rightarrow \infty$ , one can study the thermodynamic

properties using the maximum eigenvalue  $\lambda$  and corresponding left  $\langle \psi^L |$  and right  $|\psi^R \rangle$  eigenvectors of the transfer matrix  $\mathcal{T}_M$ . The free energy is determined purely by  $\lambda$ ,  $F = -(1/2\beta) \ln \lambda$ . From the derivatives of  $F$  one can in principle calculate the internal energy  $U$ , the magnetization  $M_z$ , the specific heat  $C_v$ , the spin susceptibility  $\chi$ , and other quantities. However, as it is difficult to evaluate accurately a derivative of a function in numerical calculations, we find that it is better to evaluate  $U$  and  $M_z$  directly from  $\langle \psi^L |$  and  $|\psi^R \rangle$ , and then calculate  $C_v$  and  $\chi$  from the derivative of  $U$  and  $M_z$ , respectively. For instance,  $U = \langle \hat{H} \rangle_T / N = \langle \hat{h}_1 \rangle_T = \langle \psi^L | \mathcal{T}_{h_1} | \psi^R \rangle / \lambda$ , where  $\langle \rangle_T$  is the thermal average with respect to the thermodynamic density matrix  $\rho_{\text{th}} = \exp(-\beta \hat{H}) / Z$  and  $\langle \psi^L | \psi^R \rangle = 1$  is assumed hereafter. The definition of  $\mathcal{T}_{h_1}$  is similar to that of  $\mathcal{T}_M$  subject to the decomposition. Its matrix elements can be obtained from the right-hand side of Eq. (3) by replacing  $\tau(\sigma_1^2 \sigma_2^2 | \sigma_1^1 \sigma_2^1)$  with  $\tau_{h_1}(\sigma_1^2 \sigma_2^2 | \sigma_1^1 \sigma_2^1) = \langle s_2^1 s_2^2 | \hat{h}_1 \exp(-\tau \hat{h}_1) | s_1^1 s_1^2 \rangle$ . Similarly, one can find out the relation between the magnetization  $M_z = \langle \sum_i s_i^z \rangle_T / N$  and the maximum eigenvectors of  $\mathcal{T}_M$ .

In our calculation, we fix  $\epsilon$  and increase the chain length  $2M$ . For each  $M$ , the temperature  $T = 1/\epsilon M$ . As  $M$  is small, one can find  $\lambda$ ,  $\langle \psi^L |$  and  $|\psi^R \rangle$  exactly. For large  $M$  we extend the DMRG idea to approximately but accurately find  $\lambda$ ,  $\langle \psi^L |$  and  $|\psi^R \rangle$  for a periodic time-slice chain. Figure 1 shows two configurations of the superblocks of  $\mathcal{T}_M$ . The superblock consists of two blocks, which we call renormalized blocks, in the dashed frames and two time slices. The system contains a renormalized block and one slice. The rest is thus its environment. We use  $n_s$  and  $n_e$  to label the basis states of the renormalized blocks in the system and the environment, respectively. The states of two time slices are represented by  $\sigma_1$  and  $\sigma_2$ . The elements of the right transfer matrix is denoted by  $\mathcal{T}_o(\sigma_1', n_s', \sigma_2''; \sigma_1, n_s, \sigma_2)$  or  $\mathcal{T}_e(\sigma_1', n_s', \sigma_2''; \sigma_1'', n_s, \sigma_2)$  if  $M = \text{odd}$  or even. The left transfer matrix can be obtained by transposing the right one. Therefore the superblock's  $\mathcal{T}_M$  is given by

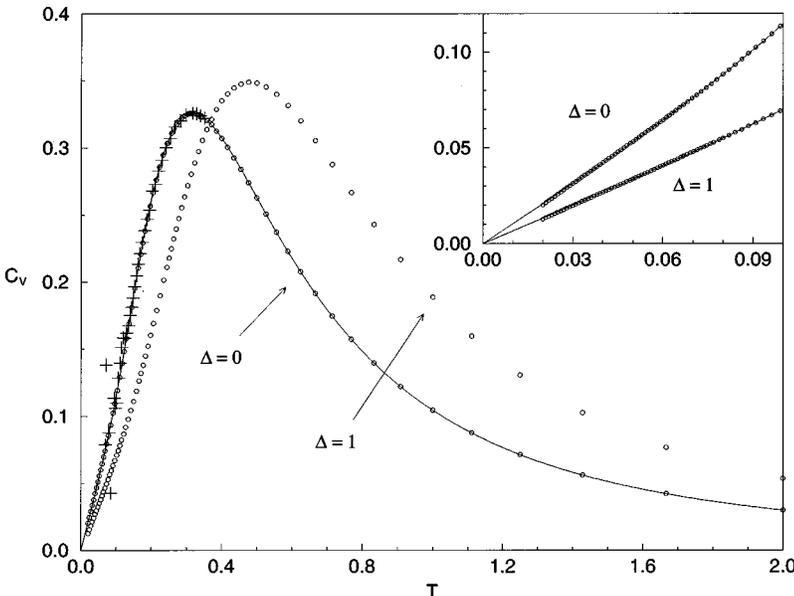


FIG. 2. The specific heat  $C_v(T)$  for both  $\Delta = 0$  and  $\Delta = 1$ . The solid curve is the exact results. Circles and pluses are the transfer matrix DMRG results with the asymmetric and symmetric density matrix, respectively.  $\epsilon = 0.05$  and  $m = 80$  are used in the transfer-matrix DMRG calculations. Inset: a polynomial fit for the low-temperature  $C_v$ .

$$\mathcal{T}_M(n'_e, \sigma'_2, \sigma'_1, n'_s; n_e, \sigma_2, \sigma_1, n_s) = \begin{cases} \sum_{\sigma''_1, \sigma''_2} \mathcal{T}_o(\sigma''_1, n_e, \sigma''_2; \sigma'_1, n'_e, \sigma'_2) \mathcal{T}_o(\sigma''_1, n'_s, \sigma''_2; \sigma_1, n_s, \sigma_2) & \text{for } M = \text{odd}, \\ \sum_{\sigma''_1, \sigma''_2} \mathcal{T}_e(\sigma_2, n_e, \sigma''_2; \sigma''_1, n'_e, \sigma'_2) \mathcal{T}_e(\sigma'_1, n'_s, \sigma''_2; \sigma''_1, n_s, \sigma_2) & \text{for } M = \text{even}. \end{cases} \quad (4)$$

To grow the chain, we have the following recursive relations:

$$\begin{aligned} \mathcal{T}_e(\sigma'_1, \tilde{n}'_s, \sigma''_2; \sigma''_1, \tilde{n}_s, \sigma_2) &= \sum_{\sigma''} \tau(\sigma'_1, \sigma' | \sigma''_1, \sigma'') \mathcal{T}_o(\sigma'', n'_s, \sigma''_2; \sigma, n_s, \sigma_2), \\ \mathcal{T}_o(\sigma''_1, \tilde{n}'_s, \sigma''_2; \sigma_1, \tilde{n}_s, \sigma_2) &= \sum_{\sigma''} \tau(\sigma''_1, \sigma'' | \sigma_1, \sigma) \mathcal{T}_e(\sigma', n'_s, \sigma''_2; \sigma'', n_s, \sigma_2), \end{aligned} \quad (5)$$

which enlarge the renormalized blocks by one slice with  $|\tilde{n}_s\rangle = |\sigma\rangle \otimes |n_s\rangle$  as the corresponding Trotter space and  $|\sigma\rangle$  as the states of a spin added. Initially, for  $2M=4$ ,  $\mathcal{T}_e(\sigma'_1, \sigma', \sigma''_2; \sigma''_1, \sigma, \sigma_2) = \sum_{\sigma''} \tau(\sigma'_1, \sigma' | \sigma''_1, \sigma'') \tau(\sigma'', \sigma''_2 | \sigma, \sigma_2)$ . As the number of states in  $|\tilde{n}_s\rangle$  exceeds  $m$ ,  $\mathcal{T}_e(\sigma'_1, \tilde{n}'_s, \sigma''_2; \sigma''_1, \tilde{n}_s, \sigma_2)$  and  $\mathcal{T}_o(\sigma''_1, \tilde{n}'_s, \sigma''_2; \sigma_1, \tilde{n}_s, \sigma_2)$  are renormalized by

$$\begin{aligned} \mathcal{T}_e(\sigma'_1, n'_s, \sigma''_2; \sigma''_1, n_s, \sigma_2) &= \sum_{\tilde{n}'_s, \tilde{n}_s} O^l(n'_s, \tilde{n}'_s) \mathcal{T}_e(\sigma'_1, \tilde{n}'_s, \sigma''_2; \sigma''_1, \tilde{n}_s, \sigma_2) O^r(\tilde{n}_s, n_s), \\ \mathcal{T}_o(\sigma''_1, n'_s, \sigma''_2; \sigma_1, n_s, \sigma_2) &= \sum_{\tilde{n}'_s, \tilde{n}_s} O^l(n'_s, \tilde{n}'_s) \mathcal{T}_o(\sigma''_1, \tilde{n}'_s, \sigma''_2; \sigma_1, \tilde{n}_s, \sigma_2) O^r(\tilde{n}_s, n_s), \end{aligned} \quad (6)$$

where the transformation matrices  $O^{l,r}$  are constructed by  $m$  truncated basis states from a reduced density matrix discussed below. Other operators such as  $\hat{h}_1$  can be renormalized by Eq. (6) with  $\tau_{h_1}$  instead of  $\tau$  in Eq. (5).

We compute the maximum eigenvalue  $\lambda$  and the corresponding right eigenvector  $|\psi^K\rangle$  of  $\mathcal{T}_M$  using a projection method. Iterating  $|\psi_K\rangle = \mathcal{T}_M |\psi_{K-1}\rangle$ , we reach  $|\psi^K\rangle = |\psi_K\rangle$  and  $\mathcal{T}_M |\psi^K\rangle = \lambda |\psi^K\rangle$  for sufficient large  $K$ .  $|\psi_0\rangle$  is an arbitrary trial vector which is not orthogonal to  $|\psi^K\rangle$ . In our calculations, we find that the value of  $K$  needed for producing an eigenvalue with a relative error less than  $10^{-16}$  is generally less than 20, but it increases with increasing  $M$ . The left eigenvector  $|\psi^L\rangle$  can be calculated similarly. However, for the systems as we study here, the wave function of  $\langle \psi^L |$  can be directly read out from the wave function of  $|\psi^K\rangle$ :  $\psi^L(n_s, \sigma_2, \sigma_1, n_e) = \psi^K(n_e, \sigma_2, \sigma_1, n_s)$  by constructing the superblocks with a reflection symmetry as involved in Eq. (4).

A density matrix for the whole system (i.e., superblock) can be defined as  $\rho = \mathcal{T}_M^{N/2} / \text{Tr} \mathcal{T}_M^{N/2}$ . This is a generalization of the thermodynamic density matrix  $\rho_{\text{th}}$  in the Trotter space. We form the reduced density matrix for the augmented renormalized block by performing a partial trace on  $\rho$  for the states of the environment

$$\rho_s = \frac{\text{Tr}_{n_e, \sigma_2} \mathcal{T}_M^{N/2}}{\text{Tr} \mathcal{T}_M^{N/2}}. \quad (7)$$

In the thermodynamic limit,  $\rho_s = \text{Tr}_{n_e, \sigma_2} |\psi^K\rangle \langle \psi^L|$ , thus the matrix element of  $\rho_s$  is given by

$$\rho_s(\tilde{n}'_s, \tilde{n}_s) = \sum_{n_e} \psi^L(\tilde{n}_e, \tilde{n}'_s) \psi^K(\tilde{n}_e, \tilde{n}_s), \quad (8)$$

with  $|\tilde{n}\rangle = |\sigma\rangle \otimes |n\rangle$ .  $\rho_s$  is an asymmetric matrix since  $\langle \psi^L | \neq (|\psi^K\rangle)^\dagger$ . The eigenvalue of  $\rho_s$  gives the probability of the corresponding eigenstates onto which the system is projected as the response to its environment. ( $|\psi^K\rangle \langle \psi^L|$  which is used to define the density matrix for the augmented system block in Ref. 11 is not a true projection operator for the maximum eigenvectors of  $\mathcal{T}_M$ .) The transformation matrices  $O^{l,r}$  in Eq. (6) are thus built up by using  $m$  left or right eigenvectors of  $\rho_s$  corresponding to  $m$  most probable eigenvalues.

Systematic errors come from two sources. One is the finiteness of  $\epsilon$ , and the other is the truncation of basis set in the DMRG iterations. The first type of error is generally very small and in principle it can be further reduced by doing an extrapolation with respect to  $\epsilon^2$ .<sup>16,17</sup> The error due to the truncation is difficult to estimate. A lower bound for this type of error is given by the truncation error  $p_m = 1 - \sum_i^m w_i$ , where  $w_i$  ( $i=1, \dots, m$ ) are the  $m$  largest eigenvalues of  $\rho_s$ . We found that  $p_m$  is generally less than  $10^{-5}$  when  $m=16$  and decreases rapidly with increasing  $m$  for the spin 1/2 system.

Figure 2 shows the results for the specific heat  $C_v(T)$  down to  $T=0.02$  with  $m=80$  and  $\epsilon=0.05$  for  $\Delta=0,1$  cases.  $C_v$  is obtained from the first derivative of  $U$ . For the XY model ( $\Delta=0$ ), we find that the relative errors are less than  $10^{-5}$  down to  $T=0.02$  for  $U$  and less than  $10^{-3}$  down to  $T=0.03$  for  $C_v$  compared with the exact results.<sup>16</sup> For the isotropic antiferromagnetic Heisenberg model ( $\Delta=1$ ), the precision of the results is similar. The maximum value of  $C_v$  is 0.3515 at  $T=0.47$ . At low temperature  $C_v$  varies linearly with  $T$ . The coefficient of the  $T$  term is shown to be  $2\theta/(3\sin\theta)$  with  $\theta = \cos^{-1}\Delta$ .<sup>18</sup> By fitting our results with a

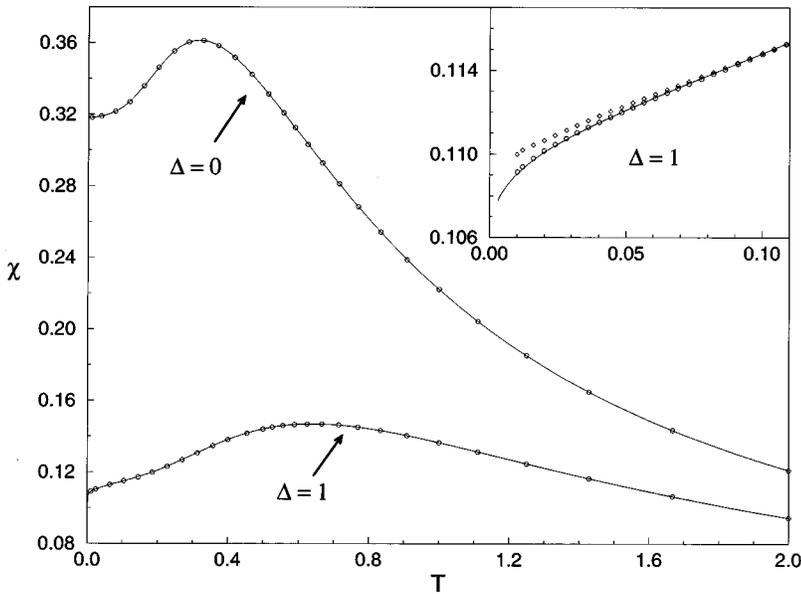


FIG. 3. The spin susceptibility  $\chi(T)$  for both  $\Delta=0$  and  $\Delta=1$ . The solid curves and circles, respectively, are the exact results (Ref. 19) and the transfer-matrix DMRG results with  $\epsilon=0.05$  and  $m=80$ . Inset compares the transfer-matrix DMRG results for  $m=32$  (diamonds) and  $80$  (circles) with the Bethe ansatz results in the low-temperature regime for  $\Delta=1$ .

polynomial up to seventh order in  $T$  for  $0.03 \leq T \leq 0.1$ , we found that the coefficients of the linear terms are 1.041 and 0.665 for  $\Delta=0$  and 1, respectively. The difference between our results and the exact ones for the linear coefficients is less than 1%.

For comparison, we also calculated  $U$  and  $C_v$  with a symmetric density matrix as defined in Ref. 11. At high temperature, the results obtained with a symmetric density matrix agree well with those obtained with an asymmetric density matrix. However, at low temperature we found that the results obtained with an asymmetric density matrix are more accurate than those obtained with a symmetric density matrix (Fig. 2). The relative errors for  $U$  and  $C_v$  obtained with the symmetric density matrix are generally larger than  $10^{-2}$  at low temperature.

Figure 3 shows our results for the spin susceptibility  $\chi(T)$  down to  $T=0.01$  with  $m=80$  and  $\epsilon=0.05$  for  $\Delta=0,1$  cases.  $\chi(T)$  is obtained from the first-order derivative of  $M_z$ , which is equal to  $M_z(T,B)/B$  for sufficient small magnetic field since  $M_z(T,0)=0$ . In our calculations,  $B=0.003$  is used. For both cases, the relative error is less than  $10^{-3}$  down to  $T=0.01$ . We note that the results of spin susceptibility are generally more accurate than those of the specific

heat. In the inset, we compare numerical results for  $\Delta=1$  with  $m=32$  and  $80$  to the exact results in the low-temperature regime. For  $m=32$  the relative error is of the order of  $10^{-3}$  at  $T=0.01$ . Our results are systematically better than those obtained by Moukouri and Caron with the thermodynamic DMRG method.<sup>14</sup>

Our computations were performed on DEC Alpha stations. It takes about 14 000 seconds on a 175 MHz station to generate a superblock size of  $2M=4000$  for  $m=32$ .

In conclusion, the quantum transfer-matrix DMRG method with asymmetric density matrices is developed. We have calculated a number of thermodynamic quantities for the anisotropic Heisenberg antiferromagnetic spin-1/2 model and found the results agree very accurately with exact ones. Our investigation shows that the transfer-matrix DMRG is a very promising method for studying thermodynamic properties of 1D quantum systems.

We are very grateful to R.J. Bursill, P. Fulde, G.A. Gehring, T. Nishino, I. Peschel, and X. Zotos for stimulating discussions, and S. Eggert and S. Moukouri for helpful correspondence. X.W. is supported by the Swiss National Fond Grant No. 933.62.186.153.

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