Thermodynamics of Strongly Correlated Systems Using the Density Matrix Renormalization Group

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I first review how the density matrix renormalization group method for the study of $T = 0$ one-dimensional strongly correlated quantum systems, has been extended to the study of the thermodynamics of two-dimensional classical and of one-dimensional quantum systems. To illustrate the method, I will show applications to frustrated quantum spin chains, which so far have defied precise numerical analysis. The incommensurability problem of exact diagonalization and the negative sign problem of quantum Monte Carlo vanish completely. The thermodynamic DMRG proves to be an extremely powerful method for the thermodynamics of frustrated systems, with promising potential for other applications.

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I. INTRODUCTION

Interest in the field of low-dimensional strongly correlated quantum systems has been enormous over the last 15 years, motivated by developments such as the discovery of the Haldane gap, one-dimensional organic superconductors, and high-T_c superconductivity. While the interest in the unobstructed observation of strong quantum effects, which characterise these systems, has focused interest on $T = 0$, the calculation of thermodynamic properties at very low, but finite temperature is highly relevant both theoretically and experimentally.

Recently, a new technique was proposed for the calculation of $T = 0$ properties of one-dimensional strongly correlated quantum systems, the density matrix renormalization group (DMRG)[1]. I will attempt to highlight the main conceptual aspects. It was then recognised that applying the DMRG concepts to transfer matrices would allow the calculation of the thermodynamic properties of two-dimensional classical[2] and, by the well-known equivalence, one-dimensional quantum systems[3]. I will explain the concepts and some of the technical aspects of this *transfer matrix* DMRG. To show the potential of the method, I will show that this method very naturally and completely eliminates the problems which made the thermodynamical properties of one-dimensional frustrated spin systems almost inaccessible in the past; the same is true for the thermodynamics of fermionic chains.

II. THE $T = 0$ DMRG ALGORITHM

Well-known numerical methods for strongly correlated one-dimensional quantum systems suffer from sometimes severe problems. Exact diagonalisation is limited to small system sizes and therefore may not capture the relevant infinite system size physics. Quantum Monte Carlo can investigate much larger systems, but low-temperature behavior, which typically contains the most interesting physics in strongly correlated systems, is hard to access. In addition, there is the (in)famous *negative sign problem*, which makes frustrated spin systems and fermionic systems virtually untreatable.

Major progress was made by the introduction of the *density matrix renormalization group* (DMRG) by White in 1992[1].

It is essentially a real space renormalization method, which linearly grows long chains: $L \to L+1$. As the size of the Hilbert space explodes, decimation is needed, to retain the most important states only. The decisive idea is to consider the system under consideration as part of an infinite size system in its ground state and to project out the environment, which gives a reduced density matrix for the system. The size of the density matrix eigenvalues shows where the most important information resides; a finite number M of the most important states is kept to describe the system. Obviously, the infinite size system is not known, but simulated by the best information available, obtained by building a large system from two copies of the system considered, one serving as environment. Iteratively, one obtains an effective low-energy Hamiltonian of a very large system.

In this way system sizes up to $L \sim 1000$ can be treated; the precision of energies is often close to machine precision. The *truncation error* $\rho = 1 - \sum_{i=1}^{M} \lambda_i$, the sum over those eigenvalues of the density matrix that were not considered, is typically less than 10^{-8}, which shows that very little information is lost. Hence the success of the method. However, all results must be extrapolated in $M \to \infty$ before the usual finite size extrapolation $L \to \infty$.

DMRG provides the lowest-lying states, their energies and correlation functions. The existence of good quantum numbers (parity, total magnetisation, total particle number), which are conserved in the DMRG iterations, allows substantial reduction of resources. However, the $T = 0$ DMRG is almost useless when it comes to the extraction of thermodynamic quantities, as it is hard to extract a sufficient number of states.

III. TRANSFER MATRIX DMRG

Decisive progress was made by Nishino's realisation that the DMRG idea could not only be used for the decimation of Hamiltonians, but also of transfer matrices[2].

Let us briefly recall the transfer matrix method for a one-dimensional classical system with Hamiltonian $\mathcal{H}$ and n states $|s_i\rangle$ on each site i, e.g. the Ising model. The first step is a local decomposition of the Hamiltonian $\mathcal{H} = \sum h_i$, where each h_i contains the interaction between sites i and $i+1$ (nearest-neighbour interactions only). Taking the partition function of a system of length L with periodic boundary conditions $L+1 \equiv 1$,

$$Z_L = \mathrm{Tr}\; e^{-\beta\mathcal{H}} = \mathrm{Tr}\; e^{-\sum_{i=1}^{L}\beta h_i}, \qquad (1)$$

and inserting identities $\sum |s_i\rangle\langle s_i|$, one obtains $Z_L = \mathrm{Tr}\;\mathcal{T}^L$, where the $n\times n$ *transfer matrix* $\mathcal{T}$ is

$$\mathcal{T} = \langle s_i|e^{-\beta h_i}|s_{i+1}\rangle.$$

From this one deduces for $L\to\infty$ the free energy per site $f = -k_B T \ln \lambda_1[\mathcal{T}]$, where λ_1 is the largest eigenvalue of $\mathcal{T}$.

Now a *twodimensional* strategy can be devised: In a two-dimensional problem of size L^2, the transfer matrix size grows as n^L. The size has to be kept finite and sufficiently small by decimation, while retaining the most important information. This is completely analogous to the conventional DMRG, with the transfer matrix replacing the Hamiltonian matrix. One therefore proceeds as follows (see Figure 1):

- The 1. dimension, having *infinite* length is attacked by the one-dimensional transfer matrix method.
- The 2. dimension, having *finite* system length is attacked by the DMRG *applied to the transfer instead of the Hamiltonian matrix.* Results are extrapolated to infinite size.

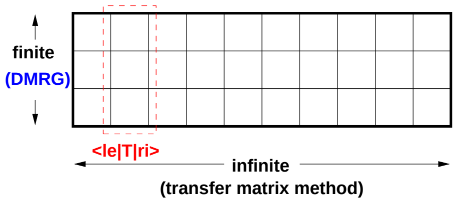

FIG. 1. Strategy for the DMRG treatment of two-dimensional classical systems.

Let us explain the DMRG transfer matrix renormalisation in somewhat more detail. Assume as given a $M\times M$ transfer matrix of a *half-system* of length L,

$$\langle m|\mathcal{T}^{(L)}|m'\rangle. \qquad (2)$$

We now build the $Mn\times Mn$ transfer matrix of the new half-system with length $L+1$ (Figure 2):

$$\langle m\, s|T^{(L+1)}|m'\, s'\rangle = \sum_{\hat{m},\hat{m}'}\langle\hat{m}|m\,\hat{s}\rangle\langle m|T^{(L)}|m'\rangle\langle\hat{s}\,s|T^{(2)}|\hat{s}'\,s'\rangle\langle m'\,\hat{s}'|\hat{m}\rangle \qquad (3)$$

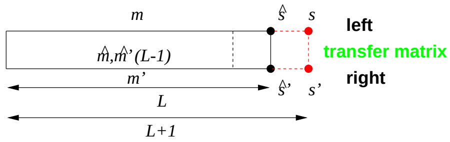

FIG. 2. Construction of enlarged transfer matrix.

The next step is the analogous construction of the $M^2n^2\times M^2n^2$ transfer matrix of the total system of length $2L+2$ (Figure 3). Lanczos diagonalisation yields the eigenvector of $\mathcal{T}^{(2L+2)}$ with the maximum eigenvalue λ_1, $|\Psi\rangle = \sum\Psi_{ij}|ij\rangle$, where $i = \{m_l s_l\}; j = \{m_r s_r\}$. This state can be used to extract the information in the half-system transfer matrices that is most pertinent to the thermodynamics of the large system. We calculate the *reduced density matrices* for half-systems $\rho_{ii'} = \sum_j \Psi_{ij}\Psi_{i'j}$. The *decimation* of half-system transfer matrices is now done by projecting the $Mn\times Mn$ half-system transfer matrices on the basis of M most important states, being the M eigenstates of the density matrix with the largest eigenvalues. Now the length of half-system is $L+1$, but the size of the transfer matrix $M\times M$ only. This procedure is repeated up to the desired final length, the free energy then obtained from λ_1.

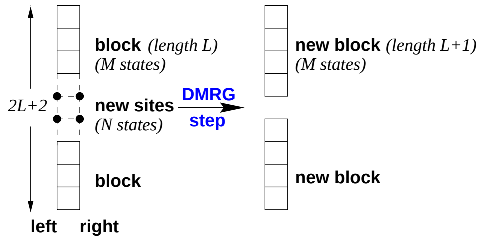

FIG. 3. Transfer matrix DMRG step.

The main technical difference between conventional DMRG and classical transfer matrix DMRG is the *absence of good quantum numbers*, which simplifies the algorithm, but is hard on computational resources.

IV. QUANTUM TRANSFER MATRIX DMRG

It is now straightforward – at least in principle – to extend the transfer matrix DMRG to the calculation of the thermodynamics of one-dimensional quantum systems[3]. To appreciate the following, it is best to visualise the DMRG as an extension of the quantum transfer matrix method in the same way the conventional DMRG extends exact diagonalisation.

One simply uses the mapping of one-dimensional *quantum* to two-dimensional *classical* systems, as used in the quantum transfer matrix (QTM)[14] and quantum Monte Carlo (QMC)[6] methods. If we use the Trotter formula

$$Z = \lim_{L\to\infty} \mathrm{Tr}\, (e^{-\beta H/L})^L = \lim_{L\to\infty} Z_L \tag{4}$$

with Trotter number L, quantum effects are suppressed as commutators are of the order L^{-2} or smaller.

We now introduce the well-known chequerboard decomposition[6] $H = H_1 + H_2$. $H_1 = \sum_i^{N/2} h_{2i-1}$ and $H_2 = \sum_i^{N/2} h_{2i}$, where h_i is the Hamiltonian linking sites i and $i+1$, are sums of local commuting Hamiltonians. N is the system size in real space (which we will take to infinity).

Then $Z_L = \mathrm{Tr}\, (e^{-\beta H_1/L} e^{-\beta H_2/L})^L$. Inserting $2L$ times the identity, we obtain a 2D lattice:

$$Z = \mathrm{Tr} \prod_{i=1}^{N/2} \prod_{j=1}^{L} \langle s_{2i-1}^{2j-1} s_{2i}^{2j-1} | e^{-\beta h_{2i-1}/L} | s_{2i-1}^{2j} s_{2i}^{2j} \rangle$$
$$\prod_{j=1}^{L} \langle s_{2i}^{2j} s_{2i+1}^{2j} | e^{-\beta h_{2i}/L} | s_{2i}^{2j+1} s_{2i+1}^{2j+1} \rangle$$

Each "spin" carries two labels, corresponding to two dimensions, the real space coordinate i and the Trotter (imaginary) space coordinate j.

Introducing a *local* transfer matrix as $\tau_k = \exp(-\beta h_k/L)$, the *global* transfer matrices

$$\mathcal{T}_1(s^1 \dots s^{2L} | t^1 \dots t^{2L}) = \prod_{j=1}^{L} \langle s^{2j-1} t^{2j-1} | \tau_1 | s^{2j} t^{2j} \rangle$$
$$\mathcal{T}_2(s^1 \dots s^{2L} | t^1 \dots t^{2L}) = \prod_{j=1}^{L} \langle s^{2j} t^{2j} | \tau_2 | s^{2j+1} t^{2j+1} \rangle$$

can be defined. One obtains

$$Z_L = \mathrm{Tr}\, [\mathcal{T}_1 \mathcal{T}_2]^{N/2}, \tag{5}$$

somewhat modified from the corresponding 2D transfer matrix DMRG expression (see Figure 4).

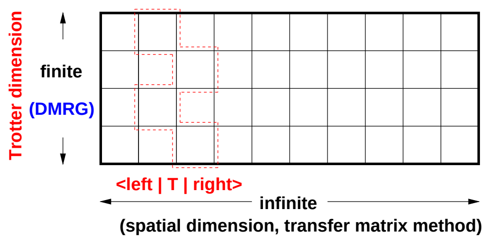

FIG. 4. Strategy for quantum transfer matrix DMRG.

Conceptually, the main steps of the algorithm are unchanged from the classical case. Formulae are slightly changed from the classical case because of the chequerboard decomposition.

At the start, the transfer matrix of two plaquettes is given by (Figure 5)

$$\mathcal{T}^3(s_0^l, s_1^l, s_1^r, s_2^r; s_0, s_2) = \sum_{s_1} \langle s_0^l s_1^l | \tau_1 | s_0 s_1 \rangle \langle s_1 s_2 | \tau_2 | s_1^r s_2^r \rangle$$

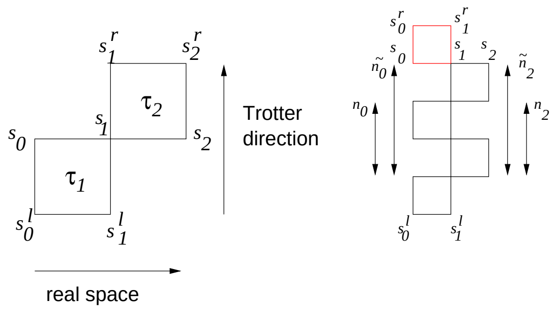

FIG. 5. Two plaquette transfer matrix and transfer matrix growth.

The addition of one plaquette reads (Figure 5):

$$\mathcal{T}^{L+1}(s_0^l, s_1^l, s_0^r, s_1^r; \tilde{n}_0, \tilde{n}_2) =$$
$$\sum_{s_1} \langle s_0 s_1 | \tau_1 | s_0^r s_1^r \rangle \mathcal{T}^L(s_0^l, s_1^l, s_1, s_2; n_0, n_2).$$

The rest of the DMRG procedure is unchanged: We build a transfer matrix of the total system and diagonalise it using Lanczos to get the maximum eigenvalue λ_1. A technical complication occurs in that the transfer matrices are asymmetric (due to the chequerboard decomposition). We therefore have to distinguish between left and right eigenvectors, and diagonalisation routines have to be monitored carefully. The density matrix derived from the eigenstate of λ_1 gives us the future basis vectors, on which we project to finish the DMRG step (see Figure 6).

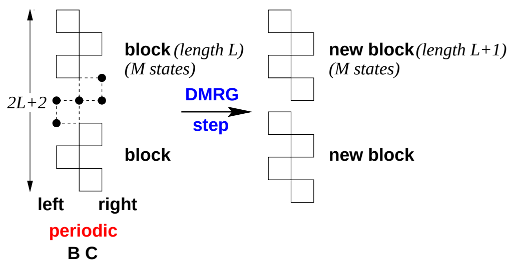

FIG. 6. Quantum transfer matrix DMRG step.

One important reduction of the computational load comes from the existence of good quantum numbers, a feature absent from the classical case. Their existence was already observed in the QTM method[7]: The action of a local Heisenberg Hamiltonian in Trotter direction between imaginary times i and $i+1$ conserves magnetisation: $[S_1^z]^{i+1} + [S_2^z]^{i+1} = [S_1^z]^i + [S_2^z]^i$, or, $[S_1^z]^{i+1} - [S_1^z]^i = -[S_2^z]^{i+1} + [S_2^z]^i$. This generalises to $\sum_i (-1)^i [S_1^z]^i = -\sum_i (-1)^i [S_2^z]^i$. Thus the staggered magnetisation, summed in *Trotter* direction, is a conserved quantity, i.e. constant along the *real space* axis:

$$Q = \sum_{j=1}^{2L} (-1)^{i+j} [S_i^z]^j = \text{cst.} \tag{6}$$

In fermionic systems, $P = \sum_{j=1}^{2L} (-1)^{i+j} [n_i]^j = \text{cst.}$ is an additional good quantum number.

A further, more technical argument shows that the good quantum numbers are conserved by the DMRG decimation process; no mixing occurs.

Moreover, the eigenstate with the maximum eigenvalue is always in the subspace $Q = 0$: Thermodynamic quantities are independent of boundary conditions. Consider open boundary conditions in real space (Figure 7).

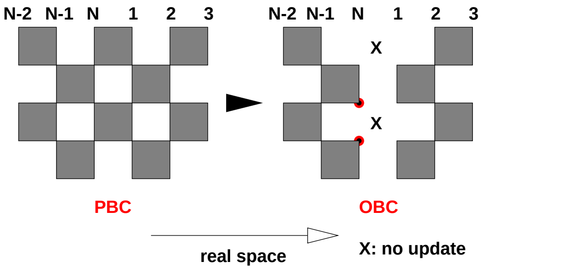

FIG. 7. Periodic vs. open boundary conditions in real space.

The incomplete update at the open ends implies the subtraction of equal quantities when forming Q, leading to $Q = 0$.

The *extraction of physical quantities* is now fairly straightforward. If we fix a β and L in (4), the transfer matrix DMRG starts at a certain initial temperature $\beta_0 = \beta/L$, reaching during its growth all multiples $n\beta_0$, up to the final β. At each step we obtain the free energy per site $f(T)$ and thus all thermodynamic quantities, such as the internal energy u, magnetisation m, specific heat at constant volume c_v, and magnetic susceptibility χ by numerical differentiation. Severe numerical problems may occur for the second order derivatives c_v and χ. A *direct* calculation of u and m, which are expectation values, reduces the number of differentiations to one.

Consider the internal energy $\langle u \rangle = Z^{-1}\text{Tr}\ [h_1 e^{-\beta H}]$. In the Trotter decomposition $\mathcal{T}_1$ changes to:

$$\mathcal{T}_u(s^1 \dots s^{2L} | t^1 \dots t^{2L}) = \tag{7}$$
$$\langle s_1^1 s_2^1 | h_1 e^{-\beta h_1} | s_1^2 s_2^2 \rangle \prod_{j=2}^{L} \langle s^{2j-1} t^{2j-1} | \tau_1 | s^{2j} t^{2j} \rangle$$

and therefore ($\langle \Psi_L |$ and $\Psi_R \rangle$ are the left (right) eigenvectors of λ_1)

$$\langle u \rangle = \frac{\text{Tr}\ [h_1 e^{-\beta H}]}{\text{Tr}\ [e^{-\beta H}]} = \frac{\langle \Psi_L | \mathcal{T}_u \mathcal{T}_2 | \Psi_R \rangle}{\lambda_1}. \tag{8}$$

Similarly, the susceptibility can be obtained with one differentiation of the magnetisation.

V. APPLICATION: FRUSTRATED QUANTUM SPIN CHAINS

For the Heisenberg chain, thermodynamic quantities can be calculated very well with the DMRG[8,9]; in fact, the results are also superior to those obtained from related attempts to apply DMRG techniques to thermodynamics[10]. However, for the systems studied, other methods had already yielded very good results[11]. Let us therefore turn to frustrated quantum spin models[12], which are both of theoretical and experimental interest, which at the moment concentrates on the famous $CuGeO_3$[13]. At the same time, they provide one of the strongest numerical challenges. We consider the spin-$\frac{1}{2}$ Hamiltonian

$$\mathcal{H} = \sum_i J_1 \mathbf{S}_{2i} \cdot \mathbf{S}_{2i+1} + J_2 \mathbf{S}_{2i-1} \cdot \mathbf{S}_{2i} + J_3 \mathbf{S}_{2i} \cdot \mathbf{S}_{2i+2} + J_4 \mathbf{S}_{2i-1} \cdot \mathbf{S}_{2i+1} + H S_i^z , \tag{9}$$

as shown in Figure 8.

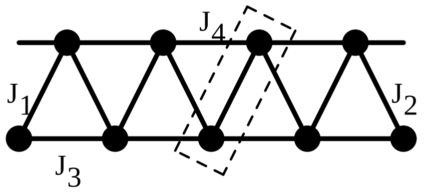

FIG. 8. Hamiltonian studied by the transfer matrix DMRG. The dashed line indicates spins grouped into a new object.

Why have other methods problems with this Hamiltonian? Exact diagonalization techniques show strong finite size effects, aggravated in frustrated systems by incommensurability effects.

Both the QTM method[14] and QMC start like the transfer matrix DMRG from the partition function $Z_m = \text{Tr}\ [e^{-\beta H_1/m} e^{-\beta H_2/m}]^m$, which becomes exact for the Trotter number $m \to \infty$. The QTM method has the advantage of working in the thermodynamic limit; however the exponential growth of the transfer matrix to be diagonalised enforces small m, a coarse Trotter decomposition, making access to low T difficult. QMC can access larger m; in frustrated spin systems, the limiting factor is the negative-sign problem: some of the matrix elements of the infinitesimal evolution operator acquire negative signs, but must be interpreted as positive probabilities. Only partial elimination of this problem has been achieved[15–18].

The modifications to the original transfer matrix DMRG for an unfrustrated antiferromagnetic chain[8,9] are very simple in principle. First, we rewrite the frustrated spin chain as a spin ladder problem. If we group two neighboring spins-$\frac{1}{2}$ into one object with 4 states, every second nearest neighbor interaction is absorbed; the others and the next-nearest neighbor interactions become effective nearest-neighbor interactions. Similar in spirit to the restructuring method of Munehisa and Munehisa[18] and Nakamura's procedure for alleviating the negative sign problem in quantum Monte Carlo[17], we are now free to choose any basis of the two-spin object which consists of eigenstates of S^z, to maintain the good quantum number Q.

For a $S = 1/2$ problem, these are essentially the Ising basis $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$ and the singlet-triplet basis $\uparrow\uparrow|\rangle$, $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$, $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$, $|\downarrow\downarrow\rangle$. Numerically, we find that both yield the same results.

The transfer matrix DMRG for frustrated spin systems combines the advantage of working in the thermodynamic limit with the disappearance of the negative sign problem and a very fine Trotter decomposition. This is because transfer matrix DMRG relates to the QZM method exactly as $T = 0$ DMRG relates to exact diagonalisation. While in QTM problems the Trotter number is of order 10, in the DMRG it increases with β, up to, say, 1000 at very low T. However, the problem of convergence in the number M of states kept has also to be considered. Working with $M \leq 32$, which is still possible on a workstation, we find that down to $T \approx 0.05$ results are very well converged; for lower T the trend is very clear (see as an example the inset of Figure 11).

In order to test the transfer matrix DMRG, we have first applied it to the so-called delta chain, because it exhibits a rather special low-temperature behavior[20], of which some approximative analytic results are known[21]. Numerical methods[15,16,20] have been applied to this chain with varying success, which makes this a good starting point for a comparison of results.

The delta chain consists of spin triangles, which are linked through the triangle basis spins ($J_1 = J_2 = J_3 = 1$, $J_4 = 0$). It has a doubly degenerate Majumdar-Ghosh ground state, with spin singlets sitting either on all left or on all right sides of the triangles[19]. Numerical studies[20] reveal that both delocalized and localized excitation are present in the system. It has been suggested that there are two types of excitations in the chain, kinks and antikinks[21,22]. Elementary excitations can be imagined as domain walls between ground state segments with a singlet on the left to singlet on the right or right to left flip. In the former case, it is energetically favorable to insert one triangle with a singlet on the basis. This is low in energy, being an eigenstate of the local triangle Hamiltonian, but localized. In the latter case, one triangle has no singlet at all, which is high in energy. However, this triangle can be delocalized. Kubo[20] has proposed that the kink and antikink excitations should lead to a second low-temperature peak in the specific heat.

We have calculated the specific heat $C_v(T)$ by numerical differentiation of the internal energy, starting from temperatures β_0 as small as 0.05, while retaining $M = 16$, 24 and 32 states, down to temperature $\beta = 40$. This implies maximum Trotter numbers up to 800.

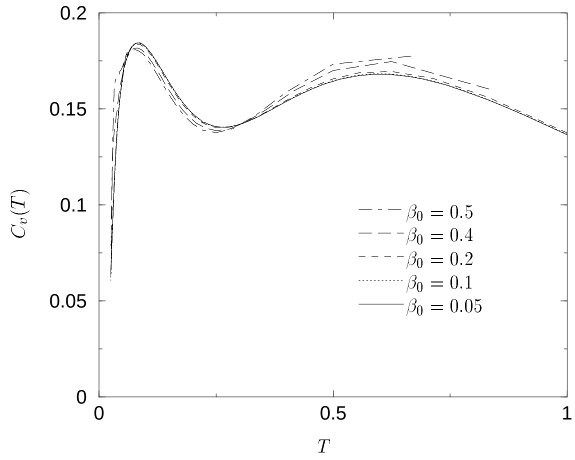

FIG. 9. Specific heat of the delta chain for 32 states kept and various β_0. Note the different convergence behavior of the high- and the low-T peak.

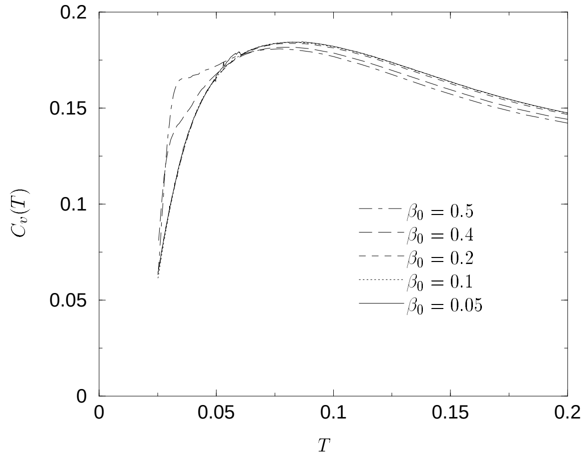

FIG. 10. Low temperature peak of the specific heat of the delta chain ($M = 32$). Curves for $\beta_0 = 0.1$ and 0.05 are almost indistinguishable.

We find that the low-temperature peak in the specific heat is converged both in β_0 and M; we extract thermodynamic limit values of $T_{peak} = 0.082(2)$ for the peak temperature and a value $C_v^{max} = 0.184(1)$. Calculating the specific heat from a variational ansatz, Nakamura and Kubo[21] predict this second peak at $T \approx 0.05$, with a height of $C_v \approx 0.24$. Numerically, Kubo finds $C_v^{max} \approx 0.18$ at $T_{peak} \approx 0.12$ from a quantum transfer method[20]; these are unextrapolated results from his maximum Trotter number. Otsuka finds $C_v^{max} \approx 0.20$ at $T_{peak} \approx 0.12$ from a recursion method[23]. Monte Carlo studies have reached the high-temperature slope of the low-T peak of C_v, but could not localize and estimate it reliably[16]. The DMRG therefore clearly gives the quantitatively most accurate results.

Let us comment on the convergence of the specific heat with $\beta_0 \to 0$. The underlying internal energy is uniformly underestimated for finite β_0, converging as β_0^2. However, as can be seen in Figure 9, for coarse Trotter slicing, the high-temperature peak is overestimated, while the low-temperature peak is underestimated. This can be understood in terms of a "sum rule": for all decompositions, $s(T=\infty) - s(T=0) = \int_0^\infty \frac{C_v(T)}{T} dT$ must be the same. Thus the errors due to the Trotter decomposition have to compensate each other.

For a comparison, the specific heat (Fig. 11) of a typical next-nearest neighbor frustrated chain (the spin-$\frac{1}{2}$ chain at its transition point $J_1 = J_2 = 1$, $J_3 = J_4 = 0.2411$) has a one-peak structure, which is converged down to $T \approx 0.04$ and can be linearly extrapolated to $C_v = 0$ at $T = 0$. For very low temperatures, the results deviate towards higher values. Comparing the curves for $\beta_0 = 0.1$ and $\beta_0 = 0.05$ indicates that the remaining error is almost entirely due to the finite number M, as the inset in Fig. 11 shows.

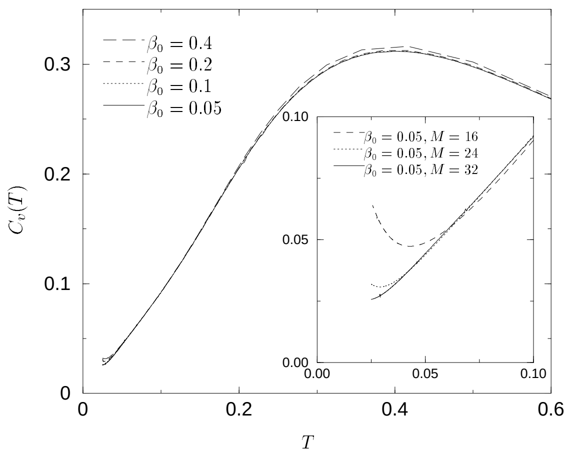

FIG. 11. Specific heat of the next-nearest neighbor frustrated spin-$\frac{1}{2}$ chain at its phase transition ($M = 32$). The inset shows the convergence with the number M of states kept of the $\beta_0 = 0.05$ curve for very low temperatures.

Similarly satisfying results can be obtained for the susceptibility (not shown).

The transfer matrix DMRG convincingly overcomes the problem of obtaining the low-temperature thermodynamics of frustrated spin chains. The method can be upgraded to more complicated frustrated chains, where other ad hoc fixtures fail. We are therefore confident that the transfer matrix DMRG will emerge as the most convenient method for obtaining the thermodynamics of frustrated spin or fermion systems.

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