Thermodynamic Density Matrix Renormalization Group Study of the Magnetic Susceptibility of Half-Integer Quantum Spin Chains

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Abstract

It is shown that White’s density matrix renormalization group technique can be adapted to obtain thermodynamic quantities. As an illustration, the magnetic susceptibility of Heisenberg $S = 1/2$ and $S = 3/2$ spin chains are computed. A careful finite size analysis is made to determine the range of temperatures where the results are reliable. For the $S = 1/2$ chain, the comparison with the exact Bethe ansatz curve shows an agreement within 1% down to $T = 0.05J$.

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One-dimensional quantum spin systems have been extensively studied for many years. In particular, a number of exact results for thermodynamic quantities were obtained for the $S = 1/2$ \cite{1} and $S = \infty$ \cite{2} systems. Unfortunately, the intermediate spin systems still offer resistance to analytical methods. The solution of the classical spin model is therefore often used to fit experimental curves. While the magnetic susceptibility $\chi$ of the $S = 5/2$ tetra-methyl manganese chloride (TMMC) was well understood using this model \cite{3}, that of CsVCl$_3$, which is a physical realization of a one-dimensional Heisenberg $S = 3/2$ chain, has shown significant discrepancy from it \cite{4} \cite{5}. Although quantum effects in a $S = 3/2$ system are expected to be weaker than in a $S = 1/2$, they are believed to be non negligible.

The purpose of this paper is to show that the density matrix renormalization group method (DMRG) \cite{6} can be applied reliably for systems at finite temperatures, the only limitation being of numerical origin at the lower temperatures. Then, after a test on the $S = 1/2$ Heisenberg chain, we will compute $\chi$ for the $S = 3/2$ chain.

Apart from the Wilson solution of the Kondo problem \cite{7}, earlier attempts to implement numerical renormalization group techniques to systems at finite temperature has led to unsatisfactorily results. Chui and Bray \cite{8} had little success on their RG study of the one-dimensional Hubbard model. A test by Hirsch \cite{9} on the simpler $S = 1/2$ Heisenberg chain led also to poor results. The advent of the DMRG has provided a framework offering new expectations. The DMRG has proven its remarkable efficiency in the calculation of the ground-state properties of many one-dimensional quantum hamiltonians. White \cite{6} showed formally that the method can easily be generalized to systems at finite temperatures. One only has to target several excited states when building the reduced density matrix. However, a straightforward application of this idea presents some difficulties. For a fixed number $m$ of states in the two largest blocks, when the number of the target states $M$ is increased, the truncation error increases. To retain good accuracy, $m$ must be at least greater than $M$. For the $S = 1/2$ Heisenberg spin chain the value of $M$ necessary to obtain the thermodynamics quantities for $T$ (in units of the exchange constant) in the range $0 - 0.5$ is roughly estimated to be several thousands for lattices of less than $N = 30$ sites. Although this value is
small compared to the number of states of the full Hilbert space, the computation of the 
$M$ states through the standard block-Lanczos or block-Davidson algorithms is impractical
because these require a very large amount of memory as well as CPU time. These difficulties
can be circumvented (non rigorously) if the $M$ states are used not for the calculation of
thermodynamic quantities but only to generate approximate hamiltonian matrices whose
sizes are kept within manageable values so as to allow complete diagonalization yet large
enough for accurate thermodynamic calculations as discussed above. In such a situation, we
found that a few tens of target states can be used to construct reliable hamiltonian matrices
that can be diagonalized using dense matrix algorithms.

We will illustrate these ideas on the one-dimensional Heisenberg model:

$$H = J S \sum_i S_i \cdot S_{i+1}$$

We will first study the case $S = 1/2$, $J_S = J = 1$. A long time ago, Bonner and Fisher
[10] computed the magnetic susceptibility of chain lengths of up to 11 sites by exact diago-
nalization. They used periodic boundary conditions (PBC) which they found to converge
much more rapidly to the infinite chain limit. Since then, the Bonner-Fisher curve is used
by experimentalists to estimate the exchange constant of physical systems. But recently, it
was noticed [11] that the results of Bonner and Fisher, while excellent at high temperatures,
turn out to deviate from the Bethe ansatz curve at lower temperatures (below $T \approx 0.2$).
This may be related to the correlation length which increases at low temperatures. As a
consequence, one needs to diagonalize longer chains. We learn from this that the method of
Bonner and Fisher would presumably lead to even worse results for systems with more than
two degrees of freedom per site.

In the DMRG, if $B$ is the block whose size is increased by one at each step and \( \bullet \)
represents an added site, then, using PBC, the superblock is $B \bullet B \bullet$. Our procedure goes
as follows: (i) We start by obtaining all the eigenvalues (through a dense matrix algorithm)
and thermodynamic averages of $BB$ with $N$ sites, which, in the first iteration, is taken to
be the largest possible ($N = 14$ in the case of $S = 1/2$ chain on our computer). Note
that this step which is necessary for the computation of thermodynamic quantities is absent in the $T = 0$ DMRG algorithm. This choice of $BB$ for the measurements instead of the superblock is motivated by the manageable size of the matrices. As usual, the states of $BB$ as well as those of the superblock are labelled by the $z$-component of the total spin and the use of parity symmetry allows us to compute only the subspaces $S^z_T = 0, 1, ...N/2$. (ii) We next build the superblock which has $N + 2$ sites. Its $M$ lowest states are computed by the block-Davidson algorithm. For a fixed $m$, $M$ is chosen to be the largest value for which the truncation error $p(m)$ is less than a desired accuracy, say $5 \times 10^{-4}$. (iii) We form and diagonalize the reduced density matrix of $B \bullet$ built from these $M$ states. We make the transformation $B = B \bullet$, and return to (i). It is important to point out that our optimization procedure in part (ii) implies, reciprocally, that it is only the $M$ targeted states that are calculated with high accuracy. It is, however, quite clear that even if only one target state is used, say the ground state of the system, the internal consistency of the DMRG is such that many of the excited states of $BB$ are also obtained with reasonable accuracy. Therefore, if many states are targeted, one expects that the excited states of $BB$ above the $M$ targeted states will be reasonably well estimated. The accuracy will, of course, certainly decrease as one goes higher in excited energy. However, the weight of these states in the partition function also decreases, thus compensating for the loss of accuracy. There is a simple test to this statement. For $m = 128$, we compared the energy of the states $M + 1, M + 2$ ...just above the cut-off $M$ (for $M = 20$) to their energies when $M$ is increased enough to include them as target states. For the case $N = 16$, the difference are in the order of $10^{-3}$ for the 5 lowest states above the cut-off. But as $M$ is further increased, the truncation error gets larger. Thus, the accuracy is reduced even on the target states if $M$ is to larger for a fixed $m$.

Let $n$ and $\Delta E_n = E_n - E_G$ be the number and the energy range of the retained eigenvalues of $BB$ respectively. $E_G$ is the ground state energy and $E_n$ is the highest eigenvalue kept of the subspace $S^z_T = 0$. To obtain good accuracy, the contribution to the partition function of the discarded eigenstates must be much smaller than that of the $n$ states. After some
steps of the DMRG, since we keep only a small fraction of states, the number of discarded
states is approximately equal to the dimension of the full Hilbert space $2^N$. Hence, at a fixed
temperature, despite the exponentially vanishing contribution of each rejected state, their
total contribution to the partition function is not necessarily negligible because of their ex-
ponentially large number. An upper bound to this contribution is roughly $2^N \exp(-\beta \Delta E_n)$. In practice we did not compute all the subspaces $S^z_T = 0, 1, \ldots N/2$; we have found that the
energies of the lowest states of the subspaces with $S^z_T \geq 7$ are higher than $E_n$ for our chosen
values of $m$ and $M$ and so these subspaces were not retained. The total number of states
involved in $BB$ for the measurements at each DMRG step is around $n = 12000$. Despite the
truncation of states in the reduced density matrix, these truncated states would contribute
mainly to form eigenvalues higher than $E_n$ in $BB$. In the present the calculations, we took,$m = 128$ and $M = 30$. The target states are distributed between the different subspaces
as follows: 10 states for the $S^z_T = 0$ subspace, 8 for $S^z_T = 1$, 4 for $S^z_T = 2$, and 2 in each
$S^z_T = 3$ to 6. This choice, which seems somewhat arbitrary, is motivated by the fact that
the subspaces having the lower $|S^z_T|$ contain the larger number of low lying states. The
largest matrix size we diagonalized was 3432. The most demanding part of the computation
obviously involved the dense matrix diagonalization of $BB$. This part of algorithm is about
50 times longer than the calculation of the $M$ states of the superblock using the Davidson
algorithm.

Fig. 1 shows the results for $\chi$ in chain of increasing even lengths from $N = 4$ up to
$N = 30$. When $N \leq 14$, the DMRG is equivalent to exact diagonalization since all the states
are kept. The truncation starts at $N = 16$ and, in this situation, the range of temperatures
where we can calculate $\chi$ with almost no finite size effects is $[\Delta E_N, T_{max}]$, where $\Delta E_N$ is the
spin gap observed at that chain length and $T_{max}$, which is the consequence of the elimination
of high lying states, is defined such that $2^N \exp(-\beta_{\max} \Delta E_n) \approx 10^{-3}$. The absence of finite
size effects (less than 0.1% when $N \geq 14$) above $\Delta E_N$ is due to the application of PBC and
to the short range nature of the interaction. In fact for a given size $N$, when $T$ is greater
than $\Delta E_N$, the value of the susceptibility is very close to that of the infinite chain. Finite
size effects start when \( T \) is in the vicinity or lower than \( \Delta E_N \). For the open boundary conditions (OBC), these would be much more significant; one would need in principle to extrapolate the results to infinity. The main advantage of the OBC is that \( p(m) \) would be smaller. As we iterate the DMRG, \( T_{\max} \) and the width \( T_{\max} - \Delta E_N \) get smaller because of the renormalization. A natural criterion when to stop the DMRG iterations appears be \( T_{\max} \lesssim \Delta E_N \). But, it should be noticed that the values of \( \chi \) for \( T \lesssim \Delta E_N \), where finite size effects are significant, are also accessible by extrapolation; the best fit is obtained with rational functions. We were able to calculate \( \chi \) down to \( T \approx 0.05 \). Below this temperature, changes in the values of \( \chi \) at each \( N \) are of the order of \( p(m) \) so that our extrapolation became unreliable. The agreement with the exact Bethe Ansatz result is quite excellent as shown in Fig 2. The DMRG curve confirms the inflection point found in ref \([11]\) at \( T = 0.087 \). The maximum deviation from the exact value is found to be less than 1%. The algorithm presented above is an infinite lattice one; the accuracy could certainly be increased by applying the finite system method \([6]\).

The same analysis is now applied to the \( S = 3/2 \) chain. In this case, there are four degrees of freedom per site. The longest chain that we were able to diagonalize exactly is \( N = 7 \). For the DMRG calculations, we took \( m = 150, p(m) \approx 7 \times 10^{-4}, M = 20 \) and the maximum chain length \( N = 16 \). We have taken 10 subspaces corresponding for the values of \( S^z_T \) ranging from 0 to 9. We retained about \( n = 20000 \) states at each step. In order to allow actual comparison with the \( S = 1/2 \) and \( S = \infty \) chains, the exchange constant and the \( g \) factor were chosen as follows: \( S^2 J_S = J/4 \) and \( Sg_S = g/2 \). The results for \( \chi \) are shown in Fig 3. The limiting susceptibility is bracketed by the curves of odd and even \( N \) obtained by exact diagonalization. We could not expect to get the same accuracy as in the \( S = 1/2 \) case since the truncation of the Hilbert space started after \( N = 6 \) only. The results for the high temperatures are not completely free of size effects. These are reduced by taking the average of \( N = 6 \) and 7. In conformity with the gapless spectrum, \( \chi \) seems to extrapolate to a finite value at \( T = 0 \). We found \( \chi = 0.12 \) at \( T = 0.04 \). But we have not made an extrapolation to \( T = 0 \); an eventual infinite slope, as for the \( S = 1/2 \) chain \([11]\), could have
been missed. We note that our results are in agreement with a recent Monte Carlo study [12]. The Monte Carlo calculation has reached a lower temperature than the present DMRG study. But, we believe that the results presented here can significantly be improved by using a powerful computer rather than our modest workstation. In Fig 4, the calculated $\chi$ of the $S = 3/2$ chain is compared with the Bethe ansatz curve of the $S = 1/2$ and Fisher’s curve of the $S = \infty$ chain. As expected, the Curie-Weiss behavior starts at lower temperature than in the $S = 1/2$ chain but at higher temperature than the classical spin.

In conclusion, we have shown that the DMRG is able to produce a static susceptibility of quantum spin chains which compares favorably with the available exact result in an extensive range of temperatures. The calculation of other thermodynamic quantities is straightforward; care must be taken to watch for finite size effects which depend on the quantity calculated. The method can presumably be used in the investigation of frustrated spin systems as well as for fermion systems such as the Hubbard or $t - J$ models; it will probably not have the difficulty that hampers the Monte Carlo method. There is a foreseeable problem when PBC are used associated with accidental degeneracies.

The calculations were made on a workstation having 128Mb memory and a speed of 25Mflops. Each DMRG step required approximately 1200 minutes.

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REFERENCES

[1] M. Takahashi, Prog. Theor. Phys. 46, 401 (1971); M. Gaudin, Phys. Rev. Lett. 26, 1301 (1971).

[2] M. E. Fisher, Am. J. Phys. 32, 343 (1964).

[3] M. T. Hutchings, G. Shirane, R. J. Birgenau and S. L. Holt, Phys. Rev. B 5, 1999 (1972).

[4] M. Niel, C. Cros, G. le Flem, M. Pouchard and P. Hegenmuller, Physica (Amsterdam) 86-88B, 702 (1977).

[5] S. Itoh, Y. Endoh, K. Kakurai and H. Tanaka, Phys. Rev. Lett. 74, 2375 (1993).

[6] S. R. White, Phys. Rev. Lett. 69, 2863 (1992); Phys. Rev. B 48, 10345 (1993).

[7] K. G. Wilson, Rev Mod. Phys. 47, 773 (1975).

[8] S. T. Chui and A. J. Bray, Phys. Rev. B 18, 2426 (1978).

[9] J. E. Hirsh, Phys. Rev. B 22, 5259 (1980).

[10] J. C. Bonner and M. E. Fisher, Phys. Rev 135, A640 (1964).

[11] S. Eggert, I Affleck and M. Takahashi, Phys. Rev. Lett. 73, 332 (1994).

[12] A. W. Sandvik and J. Kurkijärvi, Phys. Rev. B 43, 5950 (1991).
FIGURES

FIG. 1. $\chi(T)$ for $S = 1/2$ chains of $N = 4$ to $N = 30$ (full lines, from right to left). The dotted line is the envelope of these curves obtained as described in the text.

FIG. 2. DMRG versus Bethe Ansatz for $\chi(T)$ for $S = 1/2$.

FIG. 3. $\chi(T)$ for $S = 3/2$ chains of $N = 4$ to $N = 16$ (full lines, from right to left). The dotted line is the envelope of these curves.

FIG. 4. DMRG ($S = 3/2$), Bethe Ansatz ($S = 1/2$) and Fisher ($S = \infty$) curves for $\chi(T)$. 
Fig. 1

\[ \chi/N g^2 \mu_B \]
Fig. 2

\[ \chi/N g^2 \mu B \]

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Fig. 3

\[ \frac{\chi}{N g^2 \mu_B} \]

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Fig. 4

\[ \chi/N g^2 \mu_B = \frac{1}{2} \]

\[ \chi/N g^2 \mu_B = \frac{3}{2} \]

\[ \chi/N g^2 \mu_B = \frac{8}{2} \]

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