Density matrix renormalization group (DMRG) for cyclic and centrosymmetric linear chains

Manoranjan Kumar, Dayasindhu Dey, Aslam Parvej, S. Ramasesha, and Zoltán G. Soos

1 S. N. Bose National Centre for Basic Sciences, Block - JD, Sector - III, Salt Lake, Kolkata - 700098, India
2 Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560012, India
3 Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA

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The density matrix renormalization group (DMRG) method generates the low-energy states of linear systems of \(N\) sites with a few degrees of freedom at each site by starting with a small system and adding sites step by step while keeping constant the dimension of the truncated Hilbert space. DMRG algorithms are adapted to open chains with inversion symmetry at the central site, to cyclic chains and to weakly coupled chains. Physical properties rather than energy accuracy is the motivation. The algorithms are applied to the edge states of linear Heisenberg antiferromagnets with spin \(S \geq 1\) and to the quantum phases of a frustrated spin-1/2 chain with exchange between first and second neighbors. The algorithms are found to be accurate for extended Hubbard and related 1D models with charge and spin degrees of freedom.

I. INTRODUCTION

Since White introduced the density matrix renormalization group (DMRG) method and applied it to the spin-1 Heisenberg antiferromagnetic chain, the technique has been recognized to be a powerful quantitative tool for obtaining the low-energy states of spin chains and ladders or of 1D quantum cell models with charge and spin degrees of freedom. The reviews of Schollwöck and Hallberg present the DMRG method in detail. They include discussions of infinite and finite DMRG algorithms, of the underlying ideas, a careful assessment of approximations, optimization schemes, the inclusion of symmetries, and more. The reviews also discuss the scope of DMRG applications to diverse 1D systems and the relation of DMRG to other numerical and theoretical methods.

The vast majority of DMRG calculations are performed on 1D systems with open boundary conditions (OBC) and an even number of sites \(N\), as proposed by White and sketched in Fig. 1. The infinite algorithm increases the targeted superblock size by two sites per step. The system (S) and environment (E) blocks are combined into a superblock whose Hamiltonian matrix retains the same order independent of the superblock’s size. Neither the boundary conditions nor even \(N\) should matter in the thermodynamic limit, \(N \to \infty\). In practice, however, DMRG calculations are performed on finite systems and the procedure in Fig. 1 is not optimal for systems with inversion symmetry at the central site.

We discuss in this paper other ways for growing 1D systems. The DMRG algorithms in Section II retain the key steps of renormalized operators, truncation and spanning of the Fock space based on the eigenvalues and eigenvectors of the density matrix, and improving the systems block states by refining the density matrices. We mention three algorithms that differ from Fig. 1. First, open 1D chains with odd \(N\) have inversion symmetry at the central site and provide complementary information to results for even \(N\). Second, periodic boundary conditions (PBC) and translational symmetry are typically assumed in condensed phases, and DMRG can be so modified. Third, the apparently minor change of adding four instead of two sites in Fig. 1 turns out to be important for weakly coupled quantum systems in certain topologies.

DMRG has principally been applied to (a) spin chains or ladders with short-range exchange interactions and (b) to extended Hubbard models with truncated as well as long-range interactions and to related fermionic models with site energies and/or several sites per unit cell. Here we discuss spin chains using algorithms that also apply to Hubbard models. We consider chains with one spin per unit cell in the thermodynamic limit rather than ladders or chains with several spins per unit cell.

The linear Heisenberg antiferromagnet (HAF) is a
chain of spin-S sites with exchange $J > 0$ between neighbors,
\[ H_S(N) = J \sum_{r=1}^{N-1} \vec{S}_r \cdot \vec{S}_{r+1} + J_{1N} \vec{S}_1 \cdot \vec{S}_N. \] (1)

The open chain has no exchange between sites 1 and N ($J_{1N} = 0$), while the ring has $J_{1N} = J$. The $S = 1/2$ chain is a prototypical many-body problem with known exact properties in the thermodynamic limit. Haldane predicted that integer $S$ chains are gapped, as has been confirmed by DMRG and other calculations. HAFs of $S \geq 1$ sites have boundary-induced edge states that are discussed in Section III with the conventional DMRG algorithm for even $N$ and a recent algorithm for odd $N$.

The $J_1 - J_2$ model with PBC has spin-1/2 sites, $J_1$ between nearest neighbors and antiferromagnetic $J_2 > 0$ between second neighbors,
\[ H(J_1, J_2) = J_1 \sum_r \vec{S}_r \cdot \vec{S}_{r+1} + J_2 \sum_r \vec{S}_r \cdot \vec{S}_{r+2}. \] (2)

The model has been extensively studied: it is frustrated for either sign of $J_1$; it has an exact critical point $J_1/J_2 = -4$ between a ferromagnetic and singlet ground state; and a simple exact ground state at $J_1/J_2 = 2$.

The quantum phase diagram in Section IV has gapped incommensurate spiral phases with doubly degenerate singlet ground states and spin correlations of finite range as well as gapless phases with nondegenerate ground state and quasi-long-range order. The ground state degeneracy in finite PBC systems is between states that are even and odd under inversion at sites.

II. TAILORED DMRG ALGORITHMS

The general problem is a 1D chain of $N$ sites with $p$ degrees of freedom per site. Fermionic systems such as Hubbard models have $p = 4$, four states per site. Spin-$S$ chains have $p = (2S + 1)$ Zeeman levels. The dimension of the Fock space is $p^N$. The matrix can typically be resolved into sectors with specified symmetries. For example, DMRG algorithms usually conserve only $S^z$ in models that conserve the total spin $S$. Exact diagonalization (ED) is feasible up to some system size. While it is advantageous to work in small sectors, the dimension increases inexorably with $N$ and precludes the thermodynamic limit that is often sought.

As shown in Fig. 1, two sites are added per step until the desired system size $N$ is reached. Let $L$ be the dimension of the Hilbert space spanned by $H$ in the sector of interest and $m$ be the number of states kept in the system block in the truncated basis. The DMRG approximation gives constant $L' \ll L$ by truncating the Fock space of the system block and renormalizing the operators in the system block at each step. The dimension of the DMRG Fock space is $p^2m^2$ and the Hilbert space in a given $S^z$ sector is usually somewhat smaller. When a superblock of $N$ sites is reached, finite DMRG is performed by systematically and repeatedly repartitioning $N$ sites into a larger “system” block and a smaller “environment” block, and vice versa. This procedure leads to density matrices for different system sizes being obtained from the desired eigenstate of the $N$-site superblock. The accuracy, quantified by the truncation error,
\[ P(m) = 1 - \sum_{j=1}^{m} \omega_j, \] (3)

increases with $m$. The sum is over the eigenvalues $\omega_j$ of the density matrix. Typical truncation errors are in the range of $10^{-7}$ to $10^{-9}$ for $m \sim 100$ to 1000 and can be evaluated for any algorithm.

An infinite DMRG procedure for systems with PBC and even $N$ is shown in Fig. 2. Two sites are added at each step, alternately in the middle of the top and bottom chains. The motivation is symmetry and ground state properties. Correlation functions may depend on boundary conditions in systems with long-range correlations. Other starting points are possible for rings.

More extensive tailoring of the DMRG algorithm is required for Y junctions, systems of $N = 3n + 1$ sites with three arm of $n$ sites that meet at a central site. The infinite algorithm is shown in Fig. 3. The system is one arm plus the central site; the environment is the rest. The junction grows by three sites per step, and the system at one step becomes an arm at the next step. The procedure in Fig. 3 is immediately applicable to OBC chains with odd $N = 2n + 1$, which can be viewed as two arms of $n$ sites and a central site.

Weakly coupled quantum systems are challenging in general and resemble dispersion forces in some ways. The $J_1 - J_2$ model, Eq. 2 discussed in Section IV can be viewed at $J_1 \sim 0$ as two spin-1/2 HAFs on sublattices of even and odd numbered sites. The sublattice spin is $S = 0$ when $N/2$ is even, $S = 1/2$ when $N/2$ is odd. The conventional DMRG algorithm becomes unstable for $J_1/J_2 < 1/2$. Adding four instead of two spins per step restores the stability for sublattices with $S = 0$ at each site.
for even \( N \) returns \( \Gamma_0(N) < 0 \) for integer \( S \) and \( \Gamma_S(N) < 0 \) relative to \( E_0(1/2, N) \) for half integer \( S \). Since DMRG algorithms conserve \( S^z \) rather than \( S \), the most accurate results are for the GS in sectors with increasing \( S^z \) and \( \Gamma_S(N) > 0 \). The singlet (doublet) for \( \Gamma_S(N) < 0 \) is an excited state in the \( S^z = 0 \) (\( S^z = 1/2 \)) sector for integer (half integer) \( S \).

According to the nonlinear sigma model, the \( S = 1 \) chain has an effective spin \( s' = 1/2 \) at each end. The size dependence of the singlet-triplet gap is

\[
\Gamma_1(N) = (-1)^N J_c \exp(-N/\xi),
\]

where \( \xi \) is the spin correlation length in the thermodynamic limit and \( J_c \) is undetermined. The upper panel of Fig. 4 shows \( |\Gamma_1| \) as a function of system size. DMRG returns \( \xi = 6.048 \) and \( J_c = 0.7137 \), consistent with previous even-\( N \) results. The gap \( -\Gamma_1 \) for odd \( N \) agrees quantitatively with Eq. 3.

The spin density at site \( r \) is

\[
\rho(r, N) = \langle S_r^z \rangle, \quad r = 1, 2, \ldots, N.
\]

The expectation value is with respect to the state of interest in the Zeeman sector \( S^z = S \). Singlets have \( \rho(r, N) = 0 \) at all sites. SDWs in \( S \geq 1 \) chains have

FIG. 3. Schematic representation of the infinite DMRG algorithm for Y junctions with equal arms: At each step, the loop encloses the arm of the next step and the superblock contains a new site, shown as an open dot, and three arms.

FIG. 4. Upper panel: Singlet-triplet gap \( |\Gamma_1(N)| \) of \( S = 1 \) chains with OBC and \( N \) spins in Eq. 1. Lower panel: DMRG results for \( |\rho(r, N)| \) to the middle of \( S = 1 \) chains. Lines are Eq. 4 with \( \xi = 6.048 \) and \( A = 0.566 \). Even and odd \( N \) deviate from \( A \exp(-r/\xi) \) near the middle of chains.

III. EDGE STATES OF HEISENBERG SPIN CHAINS

We consider \( H_S \) in Eq. 1 and set \( J = 1 \) as the energy unit. The ground state (GS) for OBC has total spin \( S_G = 0 \) for an even number of sites \( N \) and \( S_G = S \) for an odd number of sites. There is no energy penalty for parallel spins at sites 1 and \( N \). The chain with PBC has \( J_{1N} = J \) and \( C_N \) translational symmetry. Antiferromagnetic coupling leads to the smallest possible GS spin: \( S_G = 0 \) for even \( N \) or for integer \( S \), and \( S_G = 1/2 \) for odd \( N \) and half integer \( S \). Exact results in the thermodynamic limit for \( S = 1/2 \) HAF refer to even \( N \).

The energy per site is necessarily the same in the thermodynamic limit, but odd \( N \) returns \( S_G = S \) for OBC and \( S_G = 1/2 \) for PBC. It follows that HAFs with \( S \geq 1 \) and OBC have edge states that correspond to boundary-induced spin density waves (BI-SDWs). The energy gap of edge states is

\[
\Gamma_S(N) = E_0(S, N) - E_0(0, N),
\]

where \( E_0(S, N) \) is the lowest energy in the sector with total spin \( S \). Even \( N \) leads to \( \Gamma_S(N) > 0 \). Odd \( N \) returns \( \Gamma_S(N) < 0 \) for integer \( S \) and \( \Gamma_S(N) < 0 \) relative to \( E_0(1/2, N) \) for half integer \( S \). Since DMRG algorithms conserve \( S^z \) rather than \( S \), the most accurate results are for the GS in sectors with increasing \( S^z \) and \( \Gamma_S(N) > 0 \). The singlet (doublet) for \( \Gamma_S(N) < 0 \) is an excited state in the \( S^z = 0 \) (\( S^z = 1/2 \)) sector for integer (half integer) \( S \).

According to the nonlinear sigma model, the \( S = 1 \) chain has an effective spin \( s' = 1/2 \) at each end. The size dependence of the singlet-triplet gap is

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\Gamma_1(N) = (-1)^N J_c \exp(-N/\xi),
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The spin density at site \( r \) is

\[
\rho(r, N) = \langle S_r^z \rangle, \quad r = 1, 2, \ldots, N.
\]
HAF chains with half integer \( S \geq 3/2 \) are gapless and their edges states are fundamentally different. Even chains have a singlet GS while odd chains have \( S_N = S \) and BI-SDWs with half integer \( S > 1/2 \). The even \( S = 3/2 \) chain has a gap \( \Gamma_1(N) \) that decreases faster than \( 1/N \) and has been studied\cite{18} to \( N = 192 \). Odd chains have \( -\Gamma_{3/2}(N) \) from the quartet GS to the \( S = 1/2 \) excited state, which is the first excited state in the \( S^z = 1/2 \) sector. Both gaps are shown in Fig. 6 up to \( N = 450 \). The dashed line for even \( N \) is the two-parameter fit of Ref.\cite{18} while the solid line is a two-parameter power law. The gap for odd \( N \) has larger amplitude and weaker size dependence.

The BI-SDWs of the \( S = 3/2 \) chain are also qualitatively different. Figure 7 shows the spin densities to the middle of even and odd chains. The total spin density is rigorously 1 for even \( N \) and \( 3/2 \) for odd \( N \), as required, but the BI-SDWs are not localized. The sum over all sites of the absolute spin density, \( |\rho(r,N)| = \sum_r |\rho(r,N)| \), diverges in the thermodynamic limit.

In phase BI-SDWs for odd \( N \) result in large amplitude at the middle that decreases in Fig. 6 slightly faster than \( r^{-1/2} \), while out of phase SDWs cancel for even \( N \). The spin correlation functions\cite{19,20} of the \( S = 1/2 \) and \( 3/2 \) HAFs and the size dependence of the amplitude suggest\cite{18} modeling the spin densities as

\[
\rho(r,N) = \left(-1\right)^{r-1} C_N \left( \frac{\ln B r}{r} \right)^{1/2} - \left(-1\right)^N \times \left( \frac{\ln B(N + 1 - r)}{N + 1 - r} \right)^{1/2}.
\] (8)

The amplitude \( C_N \) depends on system size because the SDWs are not localized. The lines for \( |\rho(r,N)| \) in Fig. 7 are Eq. 8 with \( B = 2 \) and the indicated \( C_N \). The spin
densities are adequately fit in the central region in either case. Deviations are limited to $r < 10$ when $N$ is even and to $r < 15$ when $N$ is odd, and such deviations are also seen in Figs. 4b and 5b for the first few sites of integer $S$ chains.

**IV. $J_1-J_2$ Model: Incommensurate and Decoupled Phases**

The $J_1-J_2$ model, Eq. [2], has been studied in several contexts. The quantum phase diagram in Fig. 8 has exact critical and special points. The thermodynamic limit at $J_2 = 0, J_1 > 0$ is a spin-1/2 HAF. The gapless phase has a nondegenerate singlet GS and spin correlations with quasi-long-range order (QLRO(\pi)) at wave vector $q = \pi$. The ferromagnetic phase with $J_1 < 0$ and LRO(0) extends to the exact critical point $P_1 = J_1/J_2 = -4$. The gapless phase at $J_1 = 0$ has QLRO(\pi/2) and corresponds to spin-1/2 HAFs on sublattices of even and odd-numbered sites. The exact GS at the Majumdar-Ghosh point, $J_1/J_2 = 2$, are doubly degenerate and very simple: They are the two Kekulé valence bond diagrams of organic chemistry in which adjacent spins are singlet paired, $(\alpha\beta - \beta\alpha)/\sqrt{2}$. The gapped dimer phase has finite-range correlations at $q = \pi$ and spontaneously broken inversion symmetry at sites. The initial studies focused on the critical point $P_4 = J_1/J_2 = 4.148$ where a singlet-triplet gap $E_{\text{in}}$ opens, the GS becomes doubly degenerate and range of spin correlations becomes finite.

The wave vector $q_G$ of GS spin correlations evolves from $q_G = 0$ at $P_1$ to $\pi$ at MG. The gapped incommensurate spiral phases have doubly degenerate GS with $\pm q_G$. The discussion so far is not at all controversial. There has been disagreement, however, about the critical points $P_2$ and $P_3$ that delimit the decoupled phase in Fig. 8. Field theories have restricted the phase to the point $J_1 = 0$ using renormalization group flows to distinguish between gapped and gapless phases. The singlet-triplet gap is very small indeed for $J_1 \sim 0$, far beyond numerical methods, and field theory also entails approximations. Another approach to the phases at small $J_1$ is to focus on GS degeneracy. The values of $P_2, P_3$ in Fig. 8 are mainly based on degeneracy.

Finite $J_1-J_2$ models of $N = 4n$ spins have discrete wave vectors that change in steps of $\pi/2n$ between $q = 0$ and $\pm \pi$ in the first Brillouin zone. The singlet GS is nondegenerate except at $2n$ values of $J_1/J_2$ between $-4$ and $2$ where it is doubly degenerate, even and odd, $\sigma = \pm 1$, under inversion at sites. The first and last degeneracy are at $J_1/J_2 = -4$ and 2, respectively, for any system size. Increasing $J_1/J_2$ generates a staircase of $2n$ steps at which $q_G$ changes by $\pi/2n$.

ED is limited to $N = 28$ in our calculations. To study larger $N = 4n$ systems, we evaluate the static structure
factor $S(q)$, with $q$ varying from 0 to $\pm \pi$ in steps of $\pi/2n$

$$S(q) = \sum_r \langle \vec{S}_0 \cdot \vec{S}_r \rangle \exp(-irq).$$  \hspace{1cm} (9)

The expectation values are in the singlet GS of systems with PBC and $-4 \leq J_1/J_2 \leq 2$. The correlation functions depend only on the separation $r$ between spins. The structure factor peaks at $q = q_G$ except in the immediate vicinity of $J_1/J_2 = 2$.

DMRG calculations yield $S(q)$ and its maximum $q_G$ as a function of $J_1/J_2$. Results to $N = 144$ are shown in Fig. 9. The line is a fit that takes into account the square-root singularities at $-4$ and $2$. The $q_G = \pi/2$ plateau is particularly important. The insets show up to $N = 192$ when the plateau is reached at $J_1/J_2 < 0$ and left at $J_1/J_2 > 0$. Linear extrapolation gives the critical points $P_2 = -1.24$ and $P_3 = 0.44$ in Fig. 8. Finite size and discrete $q$ are advantageous here since $q_G$ is exactly $\pi/2$ and the GS is nondegenerate until $q_G$ changes by $\pm \pi/2n$. The gapless decoupled phase in the interval $-1.24 \leq J_1/J_2 \leq 0.44$ requires a modest extrapolation when viewed in terms of GS degeneracy.

Okamoto and Nomura evaluated P4 by noting that a doubly degenerate GS in the dimer phase requires two singlets at lower energy than the lowest triplet. ED to $N = 24$ gave $J_1/J_2$ at which the singlet excited state and the triplet are degenerate. The weak size dependence of the crossing allowed accurate extrapolation to $P4 = 4.148$. ED$^{23}$ DMRG$^{24}$ and field theory$^{25}$ are in excellent agreement for $P4$.

ED to $N = 28$ for excited state crossings$^{24}$ also returns estimates for $P2$ and $P3$. The size dependence is stronger but entirely consistent with critical points based on GS degeneracy. As for $P4$, the singlet GS has $q_G = \pi$ for $J_1/J_2 \geq 2$ and $P4$ is related to the divergence of $S(\pi)$ in the QLRO($\pi$) phase. Spin correlations are limited to nearest neighbors at the MG point, where $S_{\text{MG}}(\pi) = 3/2$ is exact. The peak $S(\pi)$ increases for $J_1/J_2 > 2$ as the range of spin correlations increases and it diverges at $P4$ in the thermodynamic limit$^{23}$ QLRO($q_G$) phases have divergent $S(q_G)$.

The spin correlations in Eq. 9 were obtained with a DMRG algorithm for PBC. The largest separation is $r = 2n$ for $N = 4n$. Correlations in OBC systems are typically computed as close to the center as possible in order to minimize end effects; $r = 2n$ requires sites $n$ and $3n$ in systems of $4n$ spins. Significant end effects can be demonstrated in half-filled systems of free electrons. There is presumably no problem when $N$ exceeds the range of correlations. It is difficult to assess the accuracy of structure factors based on OBC spin correlations, and PBC is clearly preferable.

V. CONCLUSIONS

As summarized in Section II, there are different ways to grow 1D systems with infinite DMRG algorithms. The physics of the system rather than energy accuracy is the reason for tailored algorithms. The general DMRG methodology holds directly or with minor modification for these algorithms. Comparable truncation errors, $P(m)$ in Eq. 3, are expected and found. The scheme in Fig. 1 grows two sites per step a 1D chain with an even number of sites. The algorithm developed for Y junctions in Fig. 3 also generates a 1D chain, two sites per step, with an odd number of sites. The scheme in Fig. 2 grows a cyclic 1D chain two sites per step. Adding four instead of two sites per steps makes the conventional algorithm applicable to weakly coupled spin-1/2 chains.

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\*
manorjan.kumar@bose.res.in

† ramasesh@sscu.iisc.ernet.in
soos@princeton.edu

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