The Non-Abelian Density Matrix Renormalization Group Algorithm

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Abstract.

We describe here the extension of the density matrix renormalization group algorithm to the case where the Hamiltonian has a non-Abelian global symmetry group. The block states transform as irreducible representations of the non-Abelian group. Since the representations are multi-dimensional, a single block state in the new representation corresponds to multiple states of the original density matrix renormalization group basis. We demonstrate the usefulness of the construction via the one-dimensional Hubbard model as the symmetry group is enlarged from $U(1) \times U(1)$, up to $SU(2) \times SU(2)$.

In past years, the density matrix renormalization group (DMRG) method [1] has been extensively used to study one and two dimensional strongly correlated electron systems [2]. This method became very popular when it was realized that it enabled a level of numerical accuracy for one dimensional systems that was not possible using other methods [3].

One major drawback of DMRG is that calculations are performed in a subspace of purely Abelian symmetries, such as the $U(1)$ symmetries of total particle number and the z component of the total spin. Thus one can only obtain a few states in different total particle number and z component of total spin sectors [4]. For models where ferromagnetism emerges the situation worsens, that is, to determine magnetization, a combination of methods must be employed which will artificially raise the energy of the higher spin state [5] within the chosen z component total spin sector.

In recognizing the imperative need, to introduce a DMRG method which has a total spin quantum number naturally implemented, a number of unsuccessful attempts were previously made (e.g., for the spin 1 Heisenberg model [6] and t-t’-U model [7,8]). The most successful previous work on the application of non-trivial symmetries is the IRF-DMRG method introduced by Sierra and Nishino [9], whereby the vertex hamiltonian is first transformed into an interaction round a face hamiltonian [11], and then a variant of DMRG is applied to the IRF model. The IRF model can be chosen such that it explicitly factors out the global symmetry group. This technique has been successfully applied to the spin 1/2 Heisenberg chain and the XXZ chain with quantum group symmetry $SU_q(2)$ [9] and later, the spin 1 and spin 2 Heisenberg chains [10]. However, the IRF-DMRG method is complicated by the necessity...
to calculate the IRF weights for each interaction term in the Hamiltonian. The number of non-trivial IRF weights increases rather quickly as the magnitude of the spins in the system is increased and for a larger global symmetry group. Thus as far as we know, the IRF-DMRG has not yet been applied to any more complex models, such as a fermionic system. In the present work we show that non-Abelian symmetries can be naturally accommodated into DMRG without the need for a vertex-IRF transformation. In this form, the starting point of a calculation is the matrix elements of the single site operators which are relatively simple to calculate; the number of such elements varies inversely with the dimension of the irreducible representations of the global symmetry group, and thus is reduced for a larger global symmetry group. For example, all single site operators of a spin chain are represented as $1 \times 1$ matrices, independent of the magnitude of the actual spins. For Hubbard-type models, the number of single site basis states is reduced from four to two, corresponding to the spinon and holon states [19].

We do not attempt here to give a complete description of the DMRG algorithm, instead we refer the reader to the original description by White [1] and more recent reviews [3], and concentrate on the essential elements of the algorithm that require modification when using non-Abelian symmetries. These are the construction of tensor product basis and operators (whether it is through adding a single site to a block, or joining blocks to construct a superblock), and the truncation of block states via the reduced density matrix.

We introduce the method by way of the Lie group $SU(2)$. This symmetry is readily applicable to all quantum spin systems that can be written in a form that does not break rotational symmetry. In principle, it is not difficult to calculate eigenstates of $SU(2)$ for a finite system by using the Clebsch-Gordan transformation [12], especially in DMRG where the system is built one or two lattice sites at a time. In this construction, the tensor product of two basis vectors, labelled here by subscripts 1 and 2, is

$$|jm(j_1 j_2 \alpha_1 \alpha_2)\rangle = \sum_{m_1, m_2} C_{m_1 m_2 m}^{j_1 j_2 j} |j_1 m_1(\alpha_1)\rangle |j_2 m_2(\alpha_2)\rangle,$$

(1)

where $C_{m_1 m_2 m}^{j_1 j_2 j}$ is the Clebsch-Gordan coefficient. Here we use the notation $j$ is the total spin quantum number, $S^2|j\rangle = j(j+1)|j\rangle$, $m$ is the projection of the spin onto the $z$-axis and $(\alpha)$ is an index that encapsulates the additional labels used in DMRG (ie, to label the $\alpha$'th basis state of the given quantum numbers). Bracketed labels are not associated with a quantum number. Constructing basis states in this way in DMRG suffers from two problems. Applying this transformation involves two summations for each operator matrix element. This impacts severely on the computational effort required to construct the block, and especially the superblock, operators. Secondly, the direct application of the usual DMRG reduced density matrix to a wavefunction constructed from some $(jm)$ subspace of Eq. (1) does not commute with the $SU(2)$ generators. Indeed, the wavefunction of an $SU(2)$ invariant system represents the same physical state independent of the $z$-component of the spin, so the density matrix of the full system is

$$\rho = \sum_{m, \alpha, \alpha'} |jm(\alpha')\rangle \langle jm(\alpha)|,$$

(2)

where the wavefunction $|\Psi_m\rangle = \sum_{\alpha} \psi_{jm(\alpha)}|jm(\alpha)\rangle$ is an eigenstate of total spin, ie $S^+|\Psi_m\rangle = \sqrt{(j-m)(j+m+1)}|\Psi_{m+1}\rangle$. Using Eq. (1) and tracing over the right basis, the $SU(2)$ invariant reduced density matrix for the left block can be constructed,

$$\rho_{\alpha_1}^L(\alpha_1', \alpha_1) = \sum_{m_1, j_2, m_2, \alpha_2} \psi_{j_1 m_1(\alpha_1'}|j_2 m_2(\alpha_2)\rangle \psi_{j_1 m_1(\alpha_1}^*|j_2 m_2(\alpha_2')\rangle,$$

(3)
which acts identically on each $m_1$ component of the basis. This equation can also be directly
by adding an additional constraint to the reduced density matrix, to force each eigenstate of
the reduced density matrix to be an eigenstate of $S^2$. For $j = 0$ this reduces to the usual
DMRG density matrix. This is seen in conventional DMRG by the well known $(2j_1 + 1)$-fold
degeneracies in the reduced density matrix eigenvalues.

Despite the additional overhead of the Clebsch-Gordan transformation, this construction of $SU(2)$ invariant DMRG works well for small values of $j$, and is described further in [15].
However, further improvements are possible. The projection quantum number $m$ can be
completely eliminated using the Wigner-Eckart theorem,

$$\langle j'|m'|\alpha')|T_{M}^J|m(\alpha)\rangle = C_{m|M}\langle j'|\alpha')|T_{M}^J||j(\alpha)\rangle,$$

for the $M$’th component of an operator $T^J$ transforming as a rank $2J+1$ tensor. The quantity
$\langle j'|\alpha')|T^J||j(\alpha)\rangle$ is the reduced matrix element [12] and is independent of the projection
quantum numbers. This operator can be considered to act on a reduced basis, given by the
complete set of basis vectors $||j(\alpha)\rangle$. In this form, the superblock wavefunction for target
state $j$ can be written

$$||\Psi\rangle = \sum_{j_1,j_2,\alpha_1,\alpha_2} \psi_{j_1,j_2,\alpha_1,\alpha_2}||j_1(\alpha_1)||j_2(\alpha_2)||,$$

over a product basis given by the Clebsch-Gordan series,

$$||j_1||j_2\rangle = ||j_1 - j_2\rangle \oplus \cdots \oplus ||j_1 + j_2\rangle.$$

The reduced density matrix associated with this state is simply

$$\rho_{j_1}^J(\alpha_1') = \sum_{j_2,\alpha_2} \psi_{j_1,\alpha_1';j_2,\alpha_2} \psi_{j_1,\alpha_1';j_2,\alpha_2}^*.$$

The matrix elements of the tensor product of operators $T^{k_1} \otimes U^{k_2}$ acting on different blocks
are given by the Wigner 9j coefficients,

$$\langle j' (\alpha'_a \alpha'_2 j'_1 j'_2) ||\left[T^{k_1} \otimes U^{k_2}\right]^k ||j(\alpha_a \alpha_2 j_1 j_2)\rangle =$$

$$\begin{bmatrix}
  j_1 & j_2 & j \\
  k_1 & k_2 & k \\
  j'_1 & j'_2 & j'
\end{bmatrix}
\langle j_1' (\alpha_1') ||T^{k_1}||j_1(\alpha_1)\rangle \langle j_2' (\alpha_2') ||U^{k_2}||j_2(\alpha_2)\rangle,$$

where the $\cdots$ term is related to the 9j coefficient [12]. With this construction, all steps of
the DMRG algorithm can be performed using only the reduced basis. The importance of this
is that, unlike equation (1), there is no summation involved. The only essential difference
from the standard DMRG formulation is the quantum number dependent 9j factor multi-
plying each subspace. Thus, there is no significant computation penalty for using the $SU(2)$
formulation, as long as the 9j coefficients can be calculated efficiently. In addition, for all two
site interactions, the only two cases that appear are where one of the block operators in (8)
is the identity operator, or when block operators are combined to form a rotational invariant.
In both these cases, the 9j coefficient reduces to a single 6j coefficient.

It is worth noting that in the $SU(2)$ formulation, the basis vectors are exact eigenstates of
total spin even after the truncation. This is not true, for example, if one attempts to force the
ground state to be in a particular total spin state by adding some suitably chosen multiple of $S^2$ to the Hamiltonian. Mixing of total spin states due to numerically near-degenerate states will still occur. Calculations involving long range interactions are also affected by the lack of explicit symmetries. Using a $U(1)$ symmetric basis labelled by the $z$-component of spin only, interaction terms no longer transform as exact representations of $SU(2)$ after a truncation. This can lead to situations where, even for a large number of kept states, the ground state is a broken symmetry Néel type state [13] and only converges slowly to an eigenstate of $S^2$. It must be emphasized that this is purely an artifact of the DMRG algorithm when appropriate symmetries are not explicitly preserved.

We now have a formulation of DMRG in which the states transform as $2j + 1$ dimensional irreducible representations of $SU(2)$. However, it is clear that the general formulation is essentially independent of the details of the $SU(2)$ algebra – given an arbitrary compact global symmetry group the only modifications to the formulation is a different series expansion corresponding to Eq. (6) and coupling coefficients from Eq. (8). For example, $SO(4)$ is easy to utilize because one can make use of the isomorphism $SO(4) \simeq SU(2) \times SU(2)/\mathbb{Z}_2$, so that the $6j$ and $9j$ coefficients are simply the product of two $SU(2)$ coefficients. The component of the algorithm that is model dependent is rather small, consisting only of the reduced matrix elements of the single site operators, typically obtained via the Wigner-Eckart theorem. The $6j$ and $9j$ coupling coefficients of the algebra only appear in the construction of the blocks, in an identical way all models that admit the symmetry group. This separation of the physical aspects (the reduced matrix elements of the single site operators) and the geometric aspects (the coupling coefficients of the symmetry group) makes the method comparatively easy to apply to a range of models. This is the main advantage of the non-Abelian formulation over the IRF-DMRG. In the latter case, without a special effort to factorize the coupling coefficients, the Boltzmann weights are rather complex quantities, especially for large symmetry groups. We have applied the non-Abelian DMRG successfully to various models with global symmetries $SU(2)$, $U(1) \times SU(2)$ [16] and $SO(4)$ [14]. The $SU(3)$ case is in progress.

The computational advantage of the non-Abelian construction is two fold: (1) each reduced basis element corresponds to $2j + 1$ basis states of the old representation, thus the storage requirement for the block operators is reduced for an equivalent number of block states. (2) the superblock basis can be projected onto an exact subspace of arbitrary total spin. As well as reducing the size of the target Hilbert space, this greatly simplifies the calculation of excited states that have total spin less than the total spin of the ground state. This is very useful for investigating magnetic phase transitions [14]. For ferromagnetic target states (or more generally, target representations with a dimension greater than one), it is possible to calculate to first order the splitting of the degenerate states due to a symmetry breaking field, trivially in the case of a uniform magnetic field $h$ (where the splitting is just $hm$, for $m = -j, -j + 1, \ldots, j$), or in other cases by calculating the projection of the wavefunction and the symmetry breaking operator onto each $z$-component of spin using the Wigner-Eckart theorem (4).

A model for which the non-Abelian formulation is eminently suited is the Hubbard model [17],

$$ H = -t \sum_{<i,j>,\sigma} \left( c_{i,\sigma}^\dagger c_{j,\sigma} + \text{H.c.} \right) + U \sum_i \left( n_{i,\uparrow} - \frac{1}{2} \right) \left( n_{i,\downarrow} - \frac{1}{2} \right). \quad (9) $$

The main feature of interest in the Hubbard model is the additional charge $SU(2)$ pseudospin symmetry [18], generated by $I^+ = \sum_i (-1)^i c_{i,\uparrow}^\dagger c_{i,\downarrow}$, $I^- = \sum_i (-1)^i c_{i,\downarrow} c_{i,\uparrow}$ and $I^z = \sum_i \frac{1}{2} (n_{i,\uparrow} + n_{i,\downarrow} - 1)$. In the resulting reduced $SO(4)$ basis, the Hubbard model contains only two basis states per site, a spinon of spin 1/2 and pseudospin zero, and a holon of spin zero and
pseudospin 1/2. The single site operators are 2 × 2 matrices over this basis. Table I shows a comparison of the ground state energy for the half-filled Hubbard model for a 60 site lattice with $t = 1$, $U = 1$, for the usual $U(1) \times U(1)$ basis of number of particles and $z$-component of spin, the $U(1) \times SU(2)$ basis of number of particles and total spin $S^2 = s(s + 1)$, and the $SO(4)$ basis of total pseudospin $I^2 = i(i + 1)$ and total spin. For the case of half-filling, where the ground state is a spin and pseudospin singlet, the dimension of the representation $D$ is equal to the number of basis states that would need to be kept to achieve the same accuracy using only $U(1)$. Table I shows that the use of $SO(4)$ symmetry gives an improvement of four orders of magnitude in the cumulative truncation error and the fractional error in the ground state energy, for virtually no increase in CPU time. The main contribution to the variance in the CPU times shown arises from differences in the number of matrix-vector multiplies being performed by the eigensolver, rather than any significant difference in the CPU time per matrix-vector multiply.

Table II shows a calculation for a higher spin state, at half-filling with spin $s = 5$. In this case, the relative improvement from using $SU(2)$ symmetries is not as good. This has two causes. Firstly, the reduction in the dimension of the Hilbert space for total spin $s = 5$ versus $z$-component of spin $s_z = 5$ is not as big as for the spin zero case. Secondly, $s = 0$ is a special case in which the number of terms in the Clebsch-Gordan expansion (6) for the superblock is exactly one per block quantum number. For higher spin states, this is no longer true and the number of states in the superblock progressively increases as the target spin is increased, as each symmetry sector of the block basis appears multiple times in the superblock basis. Thus for a fixed number of states kept, the dimension of the superblock is much larger, with a corresponding increase in the CPU time.

However we note that targeting a state of spin $j$ is equivalent to inserting a non-interacting spin of magnitude $j$ into the system and targeting a state of spin zero of the combined system + non-interacting spin. Inserting this spin into the centre of the lattice, in between the system and environment blocks, is equivalent to targeting the spin $j$ state directly. If however the non-interacting spin is placed at one end of the chain and integrated into one of the blocks (it doesn’t matter which), the superblock dimensionality problem is avoided with only very minor loss of accuracy. This technique has been used before to target higher spin states in the IRF-DMRG algorithm [10]. The reflection symmetry is explicitly broken by the non-interacting spin, however the increased efficiency is well worth the loss of this symmetry. During the initial build sweep of the finite size algorithm, it is still necessary to target higher spin states because for a large enough non-interacting spin, there are not enough spins in the initial four-site block for the spin zero sector to contain any basis states [20]. For a target state of $L$ sites and spin $j$, the actual target state during the build sweep when the lattice size is $l$ sites (not counting the non-interacting spin), is $j(1 - l/L)$, rounded to the nearest permissible half-integer. Table III shows the improvement when this form of targeting is used. As this table shows, the additional superblock states that are included when the direct targeting method is used have negligible effect on the variational energy.

We have extended the DMRG algorithm so that the block and superblock basis states transform as representations of an arbitrary compact non-Abelian global symmetry group, and demonstrated the improvement in accuracy for the Hubbard model utilizing spin and pseudospin symmetry. This is a true generalization of the conventional DMRG algorithm in that, if we instead use the coupling coefficients of $U(1)$ instead of $SU(2)$ in Eq. (8), the original DMRG algorithm is recovered exactly. Thus optimizations such as efficiently storing the block operators [21], and transforming the obtained wavefunction to be the initial vector for the next DMRG iteration [22] apply to the non-Abelian case in a straightforward manner and were used in the current calculation. We have shown that, for the ground state of the
Table I – Comparison of $U(1) \times U(1)$, $U(1) \times SU(2)$ and SO(4) basis for the groundstate of the half-filled Hubbard model for a 60 site lattice, at $t = U = 1$. Number of states kept $m$, dimension of the group representation $D$, energy $E$, fractional error in the energy, cumulative truncation error over the sweep $1 - \sigma$, CPU time in seconds per sweep.

| basis          | $m$  | $D$  | $E$        | $(E - E_0)/|E_0|$ | $1 - \sigma$ | CPU    |
|----------------|------|------|------------|-------------------|--------------|--------|
| $U(1) \times U(1)$ | 100  | 200  | -61.7484986435 | 5.2x10^{-6}     | 5.3x10^{-4} | 10     |
| $U(1) \times U(1)$ | 200  | 200  | -61.7514641444 | 4.5x10^{-6}     | 4.8x10^{-5} | 41     |
| $U(1) \times U(1)$ | 300  | 300  | -61.7516910404 | 7.9x10^{-7}     | 8.8x10^{-6} | 110    |
| $U(1) \times SU(2)$ | 100  | 226  | -61.7515581914 | 2.9x10^{-6}     | 3.1x10^{-5} | 15     |
| $U(1) \times SU(2)$ | 200  | 468  | -61.7517319907 | 1.3x10^{-7}     | 1.4x10^{-6} | 64     |
| $U(1) \times SU(2)$ | 300  | 716  | -61.7517389831 | 1.4x10^{-8}     | 1.5x10^{-7} | 158    |
| SO(4)          | 100  | 526  | -61.7517351742 | 7.6x10^{-8}     | 8.4x10^{-7} | 18     |
| SO(4)          | 200  | 1136 | -61.7517397636 | 1.4x10^{-9}     | 1.5x10^{-8} | 71     |
| SO(4)          | 300  | 1766 | -61.7517398448 | 9.9x10^{-11}    | 1.0x10^{-9} | 133    |

half-filled Hubbard model, keeping only 300 $SO(4)$ states is equivalent to keeping over 1700 states of the $U(1) \times U(1)$ basis of the original DMRG formulation. As the spin of the target state is increased, the accuracy improvement diminishes because the difference between the dimension of the Hilbert space of the total spin symmetry sector and the highest weight $z$-component of spin sector is reduced. Directly targetting a higher spin state is inefficient because the Clebsch-Gordan expansion implies that the dimension of the superblock will be much larger for the same number of block states. This inefficiency can be easily overcome by using a non-interacting spin to force the target state into the singlet symmetry sector.

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Table II – Comparison of the $U(1) \times U(1)$, $U(1) \times SU(2)$ and SO(4) basis for the lowest spin 5 excited state for the half-filled Hubbard model on a 60 site lattice with $t = U = 1$.

| basis          | $m$  | $E$        | $(E - E_0)/|E_0|$ | $1 - \sigma$ | CPU    |
|----------------|------|------------|-------------------|--------------|--------|
| $U(1) \times U(1)$ | 100  | -59.5701792131 | 4.0x10^{-7}     | 3.9x10^{-4} | 11     |
| $U(1) \times U(1)$ | 200  | -59.5723270633 | 3.6x10^{-6}     | 3.8x10^{-6} | 41     |
| $U(1) \times U(1)$ | 300  | -59.5725015232 | 6.3x10^{-7}     | 6.8x10^{-5} | 102    |
| $U(1) \times SU(2)$ | 100  | -59.5702795890 | 3.8x10^{-5}     | 3.9x10^{-4} | 26     |
| $U(1) \times SU(2)$ | 200  | -59.5723402180 | 3.3x10^{-6}     | 3.7x10^{-5} | 90     |
| $U(1) \times SU(2)$ | 300  | -59.5725035338 | 5.9x10^{-7}     | 6.8x10^{-6} | 207    |
| SO(4)          | 100  | -59.5723565660 | 3.1x10^{-5}     | 3.5x10^{-5} | 32     |
| SO(4)          | 200  | -59.5725315037 | 1.3x10^{-7}     | 1.4x10^{-6} | 127    |
| SO(4)          | 300  | -59.5725381508 | 1.4x10^{-8}     | 1.5x10^{-7} | 297    |
Table III – Comparison of the $U(1) \times U(1)$, $U(1) \times SU(2)$ and $SO(4)$ basis for the lowest spin 5 excited state for the half-filled Hubbard model on a 60 site lattice with $t = U = 1$, using a non-interacting spin to target the appropriate symmetry sector.

| basis         | $m$ | $E$         | $(E - E_g)/|E_g|$ | $1 - \sigma$ | CPU |
|---------------|-----|-------------|------------------|--------------|-----|
| $U(1) \times SU(2)$ | 100 | $-59.5702385716$ | $3.9 \times 10^{-6}$ | $3.8 \times 10^{-4}$ | 14  |
| $U(1) \times SU(2)$ | 200 | $-59.5723344203$ | $3.4 \times 10^{-6}$ | $3.6 \times 10^{-6}$ | 47  |
| $U(1) \times SU(2)$ | 300 | $-59.5725027479$ | $6.1 \times 10^{-7}$ | $6.7 \times 10^{-6}$ | 113 |
| $SO(4)$        | 100 | $-59.5732497975$ | $3.2 \times 10^{-6}$ | $3.4 \times 10^{-5}$ | 16  |
| $SO(4)$        | 200 | $-59.5725312667$ | $1.3 \times 10^{-7}$ | $1.4 \times 10^{-6}$ | 64  |
| $SO(4)$        | 300 | $-59.5725381253$ | $1.4 \times 10^{-8}$ | $2.2 \times 10^{-7}$ | 148 |

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