A Two-dimensional Infinite System Density Matrix Renormalization Group Algorithm

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It has proved difficult to extend the density matrix renormalization group technique to large two-dimensional systems. In this Communication I present a novel approach where the calculation is done directly in two dimensions. This makes it possible to use an infinite system method, and for the first time the fixed point in two dimensions is studied. By analyzing several related blocking schemes I find that there exists an algorithm for which the local energy decreases monotonically as the system size increases, thereby showing the potential feasibility of this method.

There is a great need for improved numerical techniques that are able to treat two-dimensional electronic systems. Fundamental questions such as the existence of superconductivity in the 2D Hubbard and t-J models have not been resolved with present-day analytical or numerical techniques. All the commonly used numerical techniques suffer from shortcomings: exact diagonalization is limited to small lattice sizes due to the exponential growth of states with the system size. Quantum Monte Carlo calculations are unable to reach large fermion systems at low temperatures due to the “sign problem”. DMRG calculations have been very successful at treating one-dimensional systems, but accurate results are difficult to obtain for large two-dimensional systems.

It seems most likely that major improvements towards a reliable 2D technique will be made within the DMRG context. Years of effort have resulted in no progress towards solving the fermion “sign problem”. It also seems unlikely that the size of available computer memory will increase fast enough to facilitate exact diagonalization calculations for large systems. Recent DMRG studies, on the other hand, have reached the largest 2D systems reported to date. In this Communication I approach the 2D DMRG calculation from a new angle, which hopefully may encourage further research in this direction.

First the basis of standard 1D DMRG and previous 2D DMRG calculations will be reviewed. The source of the difficulties with previous 2D calculations is discussed. Thereafter several new 2D blocking schemes are proposed and tested, keeping only a small number of states per block. Finally a promising algorithm is discussed in more detail. All calculations are performed on the 2D antiferromagnetic Heisenberg model. The ground state parameters of this fundamental quantum-mechanical model are known to a high accuracy, which makes it an ideal testing ground for new numerical techniques.

The central idea in a DMRG calculation is to iteratively increase the system size, but to avoid an exponentially increasing number of states by keeping only a fixed number of the “most important” states at each iteration. In early numerical renormalization calculations the lowest eigenstates of the system were chosen to be the “important states”, but the results were discouraging. The major breakthrough came with White’s insight to use the density matrix to determine which states to keep. In the superblock method a number of blocks are combined together to form a superblock. The superblock is divided into two parts, the “system block” and the “environment block”. At each iteration the superblock is diagonalized and the density matrix is formed for the system block. The density matrix is diagonalized and the importance of each eigenstate is given by its eigenvalue. The states with the largest eigenvalues are kept and the rest discarded. In the next step of the iteration this system block, with a reduced number of states, will be used in forming the new superblock. Thus the number of sites increases with each iteration, while the number of states kept remains constant.

Using this basic formula many different DMRG algorithms can be defined. An algorithm is characterized by how the superblock is constructed, and by the manner in which the blocks are enlarged. The most commonly used method was proposed in White’s original work. The superblock consists of four blocks, with the two central blocks consisting of single sites, and the two end blocks being reflections of each other, see Fig. 1. The system block is taken to be half the superblock, that is, one end block and an adjacent single site, here called a building block. Using the density matrix a fixed number of states are kept for the system block, which in the next iteration will be recombined with a building block to form a new system block. In this manner the system blocks are enlarged by the size of the building block (here one site) at each iteration. A variation of this method is to form the superblock out of three blocks, two end blocks and a single site in the middle. The system block is chosen as above, but the environment block consists of a single end block.

If the above procedure is iterated repeatedly one can reach arbitrarily large systems. This is called the infinite system method. In the thermodynamic limit the energy does approach a fixed point, and as the number of states kept is increased, the fixed point approaches the bulk ground state energy for the model. Usually the infinite system method has been used to measure various quantities in the middle of very large systems. In this manner results with an accuracy of up to 13 digits have been reported.
The rate of convergence does depend on how the superblock is constructed. If one tries to add the building block at the outer boundary of the superblock, then the local energy will increase as one increases the system size, indicating that a good basis has not been chosen. This can easily be understood since with open periodic boundary conditions the wave function has to vanish at the boundary. If one adds a site to the boundary it is clear that some artifact will remain in the wave function as the system size is increased. This somewhat trivial example shows that one cannot construct an arbitrary blocking scheme and expect that a DMRG calculation will yield a fast convergence. This will become more evident for 2D systems.

In addition to the infinite system method discussed above, a finite system method, also introduced in White's pioneering work, is commonly used. This algorithm is used to calculate properties of finite size systems to high accuracy. Initially the infinite system method is used to reach a system of desired length \( L \). At each iteration the system block is saved, so that when a system of size \( L \) is reached, system blocks of sizes 1 to \( L/2 - 1 \) are saved. Once the desired total system size has been reached the superblock size is fixed. Next the saved system blocks are used as environmental blocks while the system block size is increased until it has reached the maximum length \( L - 3 \). Now system blocks of sizes 1 to \( L - 3 \) are saved and these blocks can be used as environment blocks for a consequent sweep through the lattice. In this manner the basis kept in the system blocks can be iteratively improved until convergence is reached.

After this brief review of 1D DMRG calculations previous 2D calculations will be considered next. Most previous 2D calculations involve mapping the 2D lattice onto a 1D system with long-range interactions.\(^5\)\(^6\)\(^7\)\(^8\)\(^9\)\(^10\)\(^11\)\(^12\) see Fig. 2. Thereafter the above 1D finite system algorithm is used. Notice that using this mapping it is not possible to use an infinite system algorithm, since one determines the size of the final lattice when doing the mapping. Also, the blocks break the symmetry of the lattice and it is generally not possible to use a reflection of the system block as the environment block. Therefore one has to use some different trick to form the environment block for the initial sweep. The two simplest options are to either leave the environment block empty, or set all long-range interactions to zero in the initial sweep. This method has, however, been able to treat the largest 2D fermion systems to date, up to sizes 11 by 16.\(^13\) An alternative approach is to add a row of sites at each iteration. In this manner strips with a width of up to 6 sites and a length of 30 sites have been studied.\(^14\)

Why have larger systems not been studied? Liang and Pang\(^11\) found that for a 2D gas of free electrons, the number of states needed to maintain a certain accuracy grows exponentially with the linear system size. This convergence was also confirmed for an algorithm were a row of sites was added at each step.\(^15\) Although no proof has been given, this statement is often referred to as most probably valid for any 2D DMRG calculation. This statement was, however, made for small finite size systems and it is not clear that it will apply to possible infinite system methods. In an infinite system DMRG calculation a fixed number of states are kept as the size of the system is increased. According to the above statement accuracy should be lost in the process. For a system with open boundary conditions the local energy decreases as the system size is increased. Furthermore, due to the variational character of the technique,\(^15\) the DMRG energy is an upper bound on the energy of the system. Therefore accuracy would certainly be lost if the DMRG energy increased as the system size is increased, in agreement with the above statement. But if the energy decreased as the system size is increased, then the bound on the system energy is continuously improved, and in the limit of the fixed point the relative accuracy will approach a constant although only a fixed number of states is kept.

It was therefore the goal of this study to investigate whether there exist 2D blocking algorithms for which the energy decreases monotonically as the system size is increased. The algorithm should retain more of the symmetry of the lattice so that it can be used in the infinite system mode, and the fixed point studied directly. The reason for the above mapping of the 2D system to a 1D system is that it is not trivial to construct such an algorithm. Since the superblock of most symmetric 2D algorithms is bound to consist of more blocks than in the 1D case computer memory limitations will also be more severe.

In order to build up a two-dimensional lattice in a more symmetric fashion it seems likely that one has to use building blocks consisting of several sites. The simplest
idea is probably to use a row of sites as building block at each iteration. This method has, however, two shortcomings; it only grows the lattice in one spatial dimension, and the number of states in the added row increases exponentially with the width of the lattice.

In a first attempt to overcome these problems I divided the square 2D lattice up into three blocks, consisting of the diagonal, a triangular block below the diagonal, and the reflection of this block above the diagonal, see Fig. 3. The lower triangular block is used as the system block, the diagonal as the building block and the reflection of the lower triangular block is used as the environment block. At each iteration the whole diagonal is thus added to the lower triangular block. In this manner one of the problems with adding just a row of sites to the system block is overcome; the lattice grows in both spatial dimensions. Furthermore, the procedure retains a high degree of symmetry and could, in principle, be used as an infinite system method. The problem is, of course, that the number of states needed to describe the exact diagonal block still increases exponentially with the linear system size. The method was, however, implemented.

When adding an exact diagonal to the system the energy per site decreased as the system size was increased, until the computer ran out of memory. Having passed this simple test the next problem to be addressed was the exponential increase of states in the diagonal. The natural way to avoid the exponential growth is to select only the most important states in the diagonal block by diagonalizing the density matrix for the diagonal. This was done, and at each iteration a single site was added in one corner. The local energy did, however, start to increase as the system size was increased. As in the 1D case, the reason seemed to be that a site was added at the boundary of the system. If periodic boundary conditions are used this may be a possible blocking formula, but it does not work with open boundary conditions.

A new method was therefore tried where, in analogy with the 1D method, the diagonal was divided into two blocks with the additional site added in the middle. The local energy did, however, still increase as a function of lattice size. A potential problem seemed to be that when working with square lattices, one is forced to construct the wave function for a lattice with an even number of sites from the wave function for a lattice with an odd number of sites. Lattices with odd and even numbers of sites do, however, have quite different wave functions. This issue can be avoided if one studies lattices tilted by 45 degrees. First an attempt was made to use lattices tilted by 45 degrees containing an even number of sites, see Fig. 4. With this geometry the standard 1D DMRG technique can be used for the diagonal, with the exception that the superblock also contains the triangular blocks. The site energy did still not decrease monotonically as the system size was increased. Therefore tilted lattices with an odd number of sites were investigated, see Fig. 5, and it was found that the energy decreased monotonically as the lattice size was increased. This was the only blocking scheme found in this study for which this was the case. The fact that there exists such an algorithm is certainly encouraging, and not self-evident, as pointed out above. Since this was the most promising algorithm found in this study the results will be analyzed in more detail next.

In Fig. 6 the site energy is shown as a function of the number of iterations. Density matrices are formed both for the diagonal and the triangular blocks, and the number of states kept in these blocks are denoted $m_d$ and $m_t$ respectively. The ground state energy for the 2D Heisenberg model is -0.669437(5). Keeping four states
in the diagonal and four blocks in the triangular block the energy levels out around -0.49. Increasing \( m_d \) to 16 dramatically improves the energy to -0.57. It seems desirable to keep a higher number of states in the diagonal than in the triangular block. Next the number of states in the triangular block was increased to eight. Then only 16 states could be kept in the triangular block, and for the number of iterations that could be done the results were slightly better than the results obtained when keeping four states in the triangular block and 16 states in the diagonal block.

![Graph showing the energy as a function of number of iterations for the 2D Heisenberg model.](image)

FIG. 6. The energy as a function of number of iterations for the 2D Heisenberg model. The number of states kept in the diagonal block is denoted \( m_d \), while the number of states in the triangular block is given by \( m_t \). The exact result is obtained from Monte Carlo simulations (Ref. 7).

In order for a DMRG method to be useful one has to be able to keep enough states per block to reach convergence in the quantity studied. Since a 2D blocking algorithm of the kind described above contains more blocks than the traditional 1D blocking method this may prove difficult. The superbloc for the above algorithm will contain \( 2m_d^2m_t^2 \) states, and the density matrix for the triangular block will contain \( 2m_d^2m_t \) states. The programs used in this investigation are, however, far from optimized. Computer memory limited the present study. By using good quantum numbers, like the \( z \)-component of the spin for the Heisenberg model, all matrices become block diagonal. In this study complete matrices were stored, and one should be able to significantly increase the number of states kept if only the non-zero matrix blocks are stored.

The important issue is thus to study how the bulk ground state energy is approached as one further increases the number of states in the blocks. The reason for the great success of the 1D DMRG method is a very fast convergence. If the 2D calculation shows exponential or power law convergence one may be able to keep enough states to reach accurate results, but if the convergence is slower this may prove difficult.

It is also possible to make a finite system algorithm based on the above blocking procedure. In such a method one could use the infinite system method for the initial steps, saving both the triangular and the diagonal blocks. Further sweeps could use these saved blocks as environment blocks and improve the basis kept in the system blocks, in a manner analogous to the 1D method.

The algorithm presented in this Communication bears some resemblance to a “four-block method” proposed by Bursill. In both methods the building block, which determines the growth of the system block, does not consist of exact sites, as in the original method, but of sites with a reduced number of states.

To conclude, using a new approach I have explored the first fully two-dimensional infinite system DMRG calculation. The fixed point in two-dimensions could be explicitly studied and it was shown that there exists an algorithm for which the local energy for the Heisenberg model decreases monotonically as the system size is increased. Previous results indicated that it is necessary to keep a number of states that grows exponentially with the linear system size to maintain a certain accuracy. This does not appear to be the case with the infinite system algorithm as the fixed point is approached. The method preserves a high degree of the symmetry of the lattice and could be used as a starting point for a finite system algorithm. Further studies are necessary to verify whether the method presented here, or other similar algorithms, exhibit convergence that is fast enough to calculate properties of large two-dimensional electronic systems.

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