Random Walk Beyond Hartree-Fock

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Abstract

We give a brief discussion of the recently developed Constrained-Path Monte Carlo Method. This method is a quantum Monte Carlo technique that eliminates the fermion sign problem plaguing simulations of systems of interacting electrons. The elimination is accomplished by trading an exact procedure for an approximate one that has been demonstrated to give very accurate estimates of energies and many-body correlation functions. We also give a short review of its applications, a discussion of several strategies for parallelizing it, and some speculation of its future extensions.

1 Introduction

We will give a brief discussion of the recently developed Constrained-Path Monte Carlo (CPMC) Method [1,2]. This ground-state ($T = 0$) method is a quantum Monte Carlo (QMC) technique that eliminates the infamous fermion sign problem plaguing simulations of systems of interacting electrons. The fermion sign problem causes the variance of measured quantities to increase exponentially with increasing system size and decreasing temperature. Rapidly the sign problem destroys one’s ability to compute with acceptable accuracy. With the CPMC method one has simulated system sizes not possible with the standard method [3]. In particular, the lattice size dependence of many-body superconducting pairing correlations functions were simulated for some of the largest lattice sizes studied to date.

In CPMC method the elimination of the sign problem is accomplished by trading an exact procedure for an approximate one that has been demonstrated to give very accurate estimates of energies and various many-body correlation functions. The exact procedure determines the lowest eigenvalue and eigenvector of the Hamiltonian by projecting them from a trial state. This

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procedure is easily converted to a branched random walk. Because of the sign problem, the random walkers carry a positive and negative weight, unfortunately in proportions such that the average weight (sign) becomes zero as the system size increases. The constrained path method is a particular way to break the symmetry in the sign of the walkers and produce only positively weighted walkers by eliminating those with a negative overlap with a certain constraining state. The procedure bears a similarly to the fixed-node Monte Carlo method [4] that has been successfully used for several decades in simulations of interacting electrons systems defined in the continuum of configuration space. The CPMC method however operates in the manifold of single-particle states (Slater determinants) defined in Fock space and hence represents quite a different and novel Monte Carlo algorithm.

In the next section we will give a brief discussion of the method. Then in the following sections will discuss the various models to which the method has been applied, highlighting significant results. After this we will discuss several strategies for parallelizing the method. At first glance it would seem as if we could simply exploit the natural parallelization enjoyed by most Monte Carlo methods [5]. In fact we need to do a bit more. In the closing section we make some speculations on future applications and extensions of the CPMC method and the potential changes in parallelization procedures.

2 The Constrained-Path Monte Carlo Method

Our numerical method is extensively described and benchmarked elsewhere [1,2]. Here we only discuss its basic strategy and approximation. In the CPMC method, the ground-state wave function $|\Psi_0\rangle$ is projected from a known initial wave function $|\Psi_T\rangle$ by a branching random walk in an over-complete space of Slater determinants $|\phi\rangle$. In such a space, we can write $|\Psi_0\rangle = \sum_\phi \chi(\phi)|\phi\rangle$.

The random walk produces an ensemble of $|\phi\rangle$, called random walkers, which represent $|\Psi_0\rangle$ in the sense that their distribution is a Monte Carlo sampling of $\chi(\phi)$, that is, a sampling of the ground-state wave function.

To completely specify the ground-state wave function for a system of interacting electrons, only determinants satisfying $\langle \Psi_0 | \phi \rangle > 0$ are needed because $|\Psi_0\rangle$ resides in either of two degenerate halves of the Slater determinant space, separated by a nodal surface $N$ that is defined by $\langle \Psi_0 | \phi \rangle = 0$. The degeneracy is a consequence of both $|\psi_0\rangle$ and $-|\psi_0\rangle$ satisfying Schrödinger’s equation. The sign problem occurs because walkers can cross $N$ as their orbitals evolve continuously in the random walk. Asymptotically they populate the two halves equally, leading to an ensemble that has zero overlap with $|\Psi_0\rangle$. If $N$ were known, we would simply constrain the random walk to one half of the space and obtain an exact solution of Schrödinger’s equation. In the constrained-
path QMC method, without \emph{a priori} knowledge of $N$, we use a trial wave function $|\Psi_T\rangle$ and require $\langle \Psi_T | \phi \rangle > 0$. This is what is called the constrained-path approximation.

The quality of the calculation clearly depends on the trial wave function $|\Psi_T\rangle$. Since the constraint only involves the overall sign of its overlap with any determinant $|\phi\rangle$, it seems reasonable to expect the results to show some insensitivity to $|\Psi_T\rangle$. Through extensive benchmarking on the Hubbard model, it has been found that simple choices of this function can give very good results \cite{1,2}.

Besides as starting point and as a condition constraining a random walker, we also use $|\Psi_T\rangle$ as an importance function. To reduce variance, we use $\langle \Psi_T | \phi \rangle$ to bias the random walk into those parts of Slater determinant space that have a large overlap with the trial state. For all three uses of $|\Psi_T\rangle$, it clearly is advantageous to have $|\Psi_T\rangle$ approximate $|\Psi_0\rangle$ as closely as possible. Only in the constraining of the path does $|\Psi_T\rangle \neq |\Psi_0\rangle$ generate an approximation.

Almost all the calculations reported here are done for square lattices with periodic boundary conditions. Mostly, we study closed shell cases, for which the corresponding free-electron wave function is non-degenerate and is translationally invariant. In these cases, the free-electron wave function, represented by a single Slater determinant, is used as the trial wave function $|\psi_T\rangle$. The use of an unrestricted Hartree-Fock wave function as $|\psi_T\rangle$ generally produces no significant improvement in the results.

We remark the the CPMC method has been extended to use generalized Hartree-Fock wave functions, of which the most famous example is the BCS wave function. The trick for doing this is described elsewhere \cite{6}.

One does simulations because exact solutions are generally unavailable, and approximate solutions, like those from Hartree-Fock approximations, are often poor. The objective of the CPMC method and other simulation methods is to go beyond Hartree Fock approximation. By expressing the wave function as a linear combination of Slater determinant, the CPMC method is a type of stochastic configuration interaction (CI) method. One difference from the classic CI method is its basis functions, the Slater determinants, being over-complete. Another difference is the set of basis states is selected via a constrained, importance-sampled random walk. There is not just one set of basis functions but many sets. Averaging over these sets is necessary to compute expectation values.
3 Applications

Except for a very recent application to a nuclear physics model [7], all applications of the constrained-path method have been to Hubbard-like models of interest to physical chemists and condensed-matter physicists. These models can be grouped as one-band, two-band, and three-band models, and each group usually has targeted classes of phenomena and materials. The Hubbard models represent considerable simplifications of the complex interactions found in actual materials but still represent complicated many-body problems for which exact solutions are rare and limited to one-dimensional systems. Under these circumstances Monte Carlo methods represent perhaps the only controlled means to study the properties of these models and benchmark approximate theories for these properties.

Hubbard models are used to study a sweeping array of intrinsically quantum many-electron phenomena. Historically these models were heavily studied for possible magnetic phenomena (ferromagnetic, anti-ferromagnetic, paramagnetic, etc.). More recently, they have been intensively studied for possible representatives of high temperature superconducting materials. In between, they were studied as candidate models of heavy fermion and mixed-valence materials.

The principal objects of interest are correlation functions, for example, spin-spin, charge-charge, pair-pair correlation functions, because the scaling of these functions with systems size gives a measure of symmetry of the ground-state. In one and two dimensions, long-range order at finite temperature is generally precluded by the Mermin-Wagner theorem. Such states however can exist at zero temperature, and their existence is signified by the behavior of correlation functions with increasing systems size. Long range anti-ferromagnetic order for example would be indicated by the \((\pi, \pi)\) peak of the Fourier transform of the spin-spin correlation function increasing with increasing system size and extrapolating to a non-zero value in the limit of infinite system size. Long-range superconducting order would be indicated by the long-range part of the pair-pair correlation function remaining a positive number as the systems size is extrapolated to infinite volume. Since the sign problem worsens as the systems size increases, having a good approximate method, like the CPMC method, is an important tool for determining whether long-range order exists in these models.
3.1 One-Band Models

The classic one-band Hubbard model is given by the Hamiltonian

\[ H = -t \sum_{\langle ij \rangle \sigma} (c_{i \sigma}^\dagger c_{j \sigma} + c_{j \sigma}^\dagger c_{i \sigma}) + U \sum_i n_{i \uparrow} n_{i \downarrow}. \]  

(1)

where the double summation is restrict to nearest neighbors, the operators \( c_{i \sigma}^\dagger \) and \( c_{i \sigma} \) create and destroy an electron of spin \( \sigma \) at lattice site \( i \), and \( n_{i \sigma} = c_{i \sigma}^\dagger c_{i \sigma} \) is the number operator at site \( i \). Typically the lattices studied have periodic boundary conditions and were square. When the interaction \( U = 0 \), the model is exactly solvable and the non-interacting electrons are described by a single band. When the number of electrons equals the number of lattice sites, the model is said to be half-filled. At half-filling \( \langle n \rangle = \langle \sum_\sigma n_{i \sigma} \rangle = 1 \).

In recent years, this model was extensively studied for its magnetic and possible superconducting properties. The half-filled model has no sign problem for most QMC methods, and QMC studies have played a major role in establishing that the ground state of the two-dimensional model has long-range anti-ferromagnetic order. This state is consistent with the observed behavior of the parent (undoped) state of high temperature superconductors. In these materials superconductivity appears when the parent state is doped away from half-filling. At dopings relevant to experiment, the sign problem is very bad. With the CPMC method it was possible to study the doped Hubbard model and to compute various correlation functions as a function of system size. The main focus has been on superconducting pairing correlation functions

To be a bit more definite, the types of correlation functions computed were: The spin density structure factor is

\[ S(k_x, k_y) = S(k) = 1/N \sum_j \exp(ik \cdot j) \langle s_0 s_j \rangle, \]  

(2)

where \( s_j = n_{j \uparrow} - n_{j \downarrow} \) is the z-component of spin at site \( j \). The charge density structure factor is similar to (2), with spin replaced by density, i.e., with the \(-\) sign in \( s_j \) replaced by a \( +\) sign. The electron pairing correlation function is defined as

\[ P_\alpha(j_x, j_y) = P(j) = \langle \Delta_\alpha^\dagger(j) \Delta_\alpha(0) \rangle, \]  

(3)

where \( \alpha \) indicates the symmetry of the pairing. The on-site \( s\)-wave pairing function has \( \Delta_s(j) = c_{j \uparrow} c_{j \downarrow} \), while for \( d\)-wave pairing we used \( \Delta_d(j) = c_{j \uparrow} \sum_\delta f(\delta) c_{j + \delta \downarrow} \), where \( \delta \) is \((\pm 1, 0)\) and \((0, \pm 1)\). For \( \delta \) along the \( x\)-axis, \( f(\delta) \) is 1; otherwise it is \(-1\).
Fig. 1. Long-range behavior of the $d_{x^2−y^2}$ pairing correlation function versus distance for $\langle n \rangle = 0.85$ and a $12 \times 12$ lattice at $U = 2, 4, \text{and } 8$ [8]. This behavior is shown for the free-electron electron and CPMC calculations. Also shown is the vertex contribution.

Simulations of the Hubbard model find that the s-wave pairing correlations are generally suppressed relative to the d-wave pairing correlations. For a given lattice size, increasing the value of $U$ suppresses the d-wave pairing and for a given value of $U$, increasing the lattice size suppresses the d-wave pairing. These results are inconsistent with long-range order and are illustrated in Figs. 1 and 2 where the d-wave pairing correlation function is shown for a $12 \times 12$ and a $16 \times 16$ lattice as a function of distance $|j|$. In these figures, also reported is the “vertex contribution” to the correlation functions defined as

$$V_{\alpha}(j) = P_{\alpha}(j) - \bar{P}_{\alpha}(j) \quad (4)$$

where $\bar{P}_{\alpha}(j)$ is the contribution of two dressed non-interacting propagators: For each term in $P_{\alpha}(j)$ of the form $\langle c_i^\dagger c_j^\dagger c_j c_i \rangle$, $\bar{P}_{\alpha}(j)$ has a term like $\langle c_i^\dagger c_j \rangle \langle c_j^\dagger c_i \rangle$. When combined, Figs. 1 and 2 indicate the likely absence of long-range superconducting order in the two-dimensional Hubbard model.

Most projector Monte Carlo ground-state calculations of Hubbard models have projected from trial states that were not superconducting. Using a trick, we projected from a d-wave BCS superconducting wave function with a BCS superconducting order parameter $\Delta = 0.5$. (Again we use the trial state not only for the initial state, but also for importance and constraining states.) Within statistical error, we found the same d-wave correlation function as we did when we projected from a free-electron wave function. One of our results is shown in Fig. 3. This similarity re-enforces the results of Ref. [8] that suggest the absence of ODLRO in the two-dimensional Hubbard model.
Adding a next-nearest neighbor hopping term of strength $t'$ to the classic Hubbard model produces the $tt'U$ model. The CPMC method has been applied to this model with the results not being materially different from those without the $t'$. Also adding the $t'$ term, whose presence is suggested by band structure calculations, does not seem to change the magnetic properties at half-filling, and away from half-filling its addition does not seem to enhance superconductivity [9,10].

Adding a nearest neighbor interaction, $V \sum \langle \langle ij \rangle \rangle n_i n_j$ with $n_i = \sum_\sigma n_{i\sigma}$, produces the $tUV$ model. The additional interaction generates additional competing effects that leading to a novel co-existence of states [11].

### 3.2 Two-Band Model

The two-band model is almost always called the periodic Anderson model. In this model a $d$ and a $f$ orbital are on each lattice site. These two orbitals per unit cell lead to two bands. The Hamiltonian is

$$H = -t \sum_{\langle ij \rangle, \sigma} (d_{i,\sigma}^d d_{j,\sigma} + d_{j,\sigma}^d d_{i,\sigma}) + V \sum_{i, \sigma} (d_{i,\sigma}^f f_{i,\sigma} + f_{i,\sigma}^f d_{i,\sigma})$$

$$+ \epsilon_f \sum_{i, \sigma} n_{i,\sigma}^f + \frac{1}{2} U \sum_{i, \sigma} n_{i,\sigma}^f n_{i,-\sigma}^f$$

where the creation and destruction operators create and destroy $d$-electrons on sites of a square lattice and $f$-electrons on localized orbitals associated

![Fig. 2](image-url) Long-range behavior of the $d_{x^2-y^2}$ pairing correlation function versus distance for $\langle n \rangle = 0.85$ and a $16 \times 16$ lattice at $U = 2$ and $4$ [8]. This behavior is shown for the free-electron electron and CPMC calculations. Also shown is the vertex contribution.
Fig. 3. Pairing correlation functions in the $d_{x^2-y^2}$-wave channel given by the CPMC method for a $10 \times 10$ lattice, $U = 4$, and $\langle n \rangle = 0.82$. The inset shows the long range part in detail. The results are the same for the two different trial wave functions: the correlations decay quickly with distance [6]. On the other hand the BCS trial wave function exhibits ODLRO. Errors bars are smaller than the size of the symbols.

with these sites. $n_{i,\sigma}^f = \hat{f}_{i,\sigma}^\dagger \hat{f}_{i,\sigma}$ is the number operator for $f$-electrons. Hopping only occurs between between neighboring lattice sites (-$t$ term) and between a lattice site and its orbital ($V$ term).

Because of the two bands, the model is half-filled when there are two electrons per lattice site. At half-filling the model is said to be symmetric when $\epsilon_f = -U/2$. For the symmetric model there is no sign problem and standard QMC methods suggest that the model is an insulating antiferromagnetic if $U > U_c \approx 2$. With the CPMC method studying the magnetic properties of the doped model was possible.

Upon doping with holes, the long-range anti-ferromagnetic order was rapidly destroyed. Around three-quarters filling of the lower band, a strong peak developed at the $(\pi,0)$ value of the spin structure factor $S_{\parallel}(k)$ for the $f$-electrons. This peak is shown in Fig. 4, and its development is consistent with the resonance of two degenerate spin-density waves with wave vectors $(\pi,0)$ and $(0,\pi)$ [12]. Unestablished is whether this novel state is one of long-range order.

3.3 Three-Band Model

The three-band model was constructed with the structure of high-temperature superconductors in mind. The common structural feature of these materials are $CuO_2$ planes. In addition, these materials possess strong two-dimensional-like anisotropy. These properties have focused attention on the physics in these planes as being the source of the superconductivity.
The three-band model studied by the CPMC method represents the Hamiltonian for the CuO$_2$ planes with only the most relevant Cu and O being kept.

$$\begin{align*}
H &= \sum_{<j,k>} t_{jk}^{pp} (p_{j\sigma}^\dagger p_{k\sigma} + p_{k\sigma}^\dagger p_{j\sigma}) + \epsilon_p \sum_j n_j^p + U_p \sum_j n_j^p n_{j\downarrow}^p \\
 &\quad + \epsilon_d \sum_i n_{i\sigma}^d + U_d \sum_i n_{i\uparrow}^d n_{i\downarrow}^d \\
 &\quad + V_{pd}^{pd} \sum_{<i,j>} n_i^d n_j^p + \sum_{<i,j>\sigma} t_{ij}^{pd} (d_{i\sigma}^\dagger p_{j\sigma} + p_{j\sigma}^\dagger d_{i\sigma})
\end{align*}$$

In writing the Hamiltonian, we adopted the convention that the operator $d_{i\sigma}^\dagger$ creates a hole at a Cu $3d_{x^2-y^2}$ orbital and $p_{j\sigma}^\dagger$ creates a hole in an O $2p_x$ or $2p_y$ orbital. $U_d$ and $U_p$ are the Coulomb repulsions at the Cu and O sites respectively, $\epsilon_d$ and $\epsilon_p$ are the corresponding orbital energies, and $V_{pd}$ is the nearest neighbor Coulomb repulsion. As written, the model has a Cu-O hybridization $t_{ij}^{pd} = \pm t_{pd}$ with the minus sign occurring $j = i + \hat{x}/2$ and $j = i - \hat{y}/2$ and also hybridization $t_{jk}^{pp} = \pm t_{pp}$ between oxygen sites with the minus sign occurring for $k = j - \hat{x}/2 - \hat{y}/2$ and $k = j + \hat{x}/2 + \hat{y}/2$. The lattice is a planar CuO$_2$ structure which has three atoms, one Cu and two O, per unit cell. Hence the non-interacting problem has three bands. In a bit of a switch, convention for this model has half-filling corresponding to half-filling of the anti-bonding (upper) band which is the lowest band in the hole representation. When the Hamiltonian is expressed in a hole representation, half-filling then corresponds to one hole per unit cell.

The superconducting pairing correlation functions were studied with the CPMC method, and the findings were similar to those found from the studies on the Hubbard model: d-wave correlations are stronger than the s-wave ones [13].
Table 1
Comparison of the exact ground-state energy with the CPMC result with a one and two Slater determinant trial wave function for a $2 \times 2$ system. Parameters are $\epsilon = \epsilon_p - \epsilon_d = 3$ and $t_{pp} = U_p = 0$. The use of two Slater determinants as described in the text improves the accuracy by an order of magnitude or more [13].

| $U_d$ | CPMC 1SD       | CPMC 2SD       | Exact           |
|-------|----------------|----------------|-----------------|
| 1     | -5.0613(3)     | -5.0764(2)     | -5.076977       |
| 2     | -4.8475(9)     | -4.8789(7)     | -4.880047       |
| 4     | -4.6073(9)     | -4.6615(6)     | -4.661723       |
| 6     | -4.4884(9)     | -4.5468(6)     | -4.547436       |

For a given system size, increasing $U$ suppress the pairing correlations. For a given $U$, increasing the system size suppresses the pairing correlations.

For the three-band model the binding energy between two holes was also calculated. This is a difficult calculation because it requires the accurate calculation of the difference between nearly equal energies. It is a significant calculation because the binding of holes is a pre-requisite for superconductivity, phase separation, or stripe formation.

To calculate the binding energy for holes, we need to study the half-filled case and then the 1 and 2 hole doped cases. In the systems considered ($2 \times 2$, $4 \times 2$ and $6 \times 4$ unit cells) the 2 hole doped case corresponds to a closed shell case. The one hole case is one hole away from a closed shell, and the corresponding free-electron wave function is doubly degenerate. In this one-hole case the accuracy of the energy is as good as in the closed shell case independently of the trial wavefunction used. However, for the half-filled case, which is two holes away from a close shell, there are 4 degenerate free-electron states. If we used a trial state made from selecting arbitrarily any one of the degenerate states or an arbitrary linear combination of these states, the calculated energies would not be accurate enough to compute the binding energy. Therefore, we used the following procedure for the half-filled case: we diagonalized the interacting part of the Hamiltonian in this degenerate subspace, and obtained 2 states with energy proportional to $U_d$ and 2 states with zero energy. Of the 2 states with zero energy only one of them is a singlet. We used this state which is represented by a linear combination of two Slater determinants: $(c_{k_1,\uparrow}c_{k_1,\downarrow} - c_{k_2,\uparrow}c_{k_2,\downarrow})|CS\rangle/\sqrt{2}$. In Table 1, we compare the energies obtained using the CPMC with the one and two Slater determinants trial wave function and energies obtained from exact diagonalization. We see that using two Slater determinants improves the accuracy by an order of magnitude or more. The accuracy has become better than the closed shell case.

With this increased accuracy we found parameter ranges where holes bind, values of the parameters where binding is optimal, and an increase in binding
energy with an increase in system size. Since the appearance of hole binding seems decoupled from any enhancement of superconducting correlation, an open question is the significance and consequence of this binding.

4 Parallelization

If we are considering a system of $N_e$ electrons and $N$ lattice sites, the CPU time scales as $N_w N_e N^2$ where $N_w$ is the number of walkers. (The number of walkers is typically of the order of 200 to 1000 with the larger number usually need for the larger values of the interaction strengths.) This number needs to be sufficiently large to insure an adequate approximation to the ground state and is determined on the basis of experience. The factor $N_e N^2$ comes from the scaling of the basic matrix operation that must be performed: The basic matrix operations are matrix multiplication, inversion, re-orthogonalization, and rank-one updates of matrix inverses. The dominant operation is the matrix multiplication propagating a walker. The propagator is represented by a $N \times N$ matrix, and each walker by two $N \times N_\sigma$ matrices, i.e., one for each spin.

In general the method is CPU intensive as opposed to memory intensive. As a consequence, the basic code usually fits in the memory of one processor and the parallelization of the simulation can follow one of several natural paths. The simplest path is to give each processor a copy of the code, have it read different independent input files, and compute independent runs. A less embarrassing parallelization, and a run time reducing one, is to share the number of walkers as equally as possible among as many processors as possible, propagate the walkers on each processor independently, and combine the results. The branched nature of the random walk however requires a slightly different procedure.

Each walker carries a weight, and as the walker propagates, its weight increases or decreases. Eventually the large weighted walkers dominate, but propagating one of them costs as much computing time as it does to propagate a small weighted walker that has little bearing on the final results. Hence carrying the small weighted walkers becomes inefficient. In these types of random walks, a standard procedure is periodically eliminating walkers with small weights and replacing each large weighted walker by many medium weighted walkers whose total weight on the average is the same as the single walker. There are several schemes to do this, and these procedures are called population control. Population control prevents a single walker from ultimately dominating the simulation and when used properly reduces the variance of the computed results.

After a population control step, the loads on the processors are unbalanced.
The natural action then would be to redistribute the load. Unless this load represents a relatively large number of walkers per processor, a danger of introducing a bias into the simulation exists by performing population control on a population too small to be representative. Such a case is expected if several hundred walkers distributed across a hundred or so processors.

Two other options for parallelization are easy to implement. One is to use relatively few well-populated processors and have them independently execute population control. (This is the procedure we used for small and intermediate lattice sizes.) The other, which is more effective in reducing run time for larger jobs when a large number of processors are available, is doing population control by moving all the walkers onto one processor, performing population control there, and then uniformly re-distributing the population. Because the amount of information passed between processors is small and the amount of time needed for population control is small, this procedure still achieves a nearly linear reduction in computation time with the number of processors and is simple to implement in any message passing environment.

5 Concluding Remarks

The constrained-path method has provided simulators of interacting electron systems with a useful tool to study systems sizes impossible by other means. With this method it has been possible to investigate the timely and important question of the nature of superconducting pairing correlations in candidate models for high temperature superconductivity. The results obtained strongly suggest the absence of long-range order in these models even though they do not provide a rigorous proof of this absence.

While appearing similar to the fixed-node method long used for continuum problem, it is not a fixed node method [14]. Appearing about the same time as the CPMC method was a lattice version of the fixed-node method [15,16]. The CPMC method appears to give more accurate estimates of quantities like the energy and correlation functions, but the fixed-node method can more easily propagate some special trial states not expressible as a sum of single Slater determinants.

The concept of constrained random walks has lead to two other quantum Monte Carlo methods. One is a constrained random walk at finite temperatures [10]. The initial results are promising. The significance is that finite temperature methods have lacked effective analogs even of the fixed-node method [17]. The other advance is the constrained phase method. The method allows for the propagators and Slater determinants to be complex valued: One has generalized the sign problem to a phase problem. The ground-state wave
functions of a system of electrons in a magnetic field must be complex-valued. Making the propagator complex-valued may be convenient if the system has long-range forces. Preliminary results on small systems in a magnetic field are also promising.

The 16 × 16 lattices size is most likely the largest for which the simple parallelization scheme described above is convenient. Often \( N_e \approx N \) so the computation scales roughly as \( N^3 \). Thus simulating a 20 × 20 system increases the run time by a factor of 4 relative to the 16 × 16 system. This increases the simulation time from 2 weeks, for example, to 2 months. It is becoming clear that one might need to simulate larger lattice sizes to insure finite-size effects are not influencing the results. Going to these larger systems will require distributing the matrix operations across many processors. Such operations are all fundamental, and procedures for doing this type of parallelization exist. We will be exploring their utilization in the near future.

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