Simulating ‘Complex’ Problems with Quantum Monte Carlo

Lizeng Zhang\textsuperscript{1,2}, Geoff Canright\textsuperscript{1,2} and Ted Barnes\textsuperscript{1,3}

\textsuperscript{1}Department of Physics and Astronomy, 
\textit{The University of Tennessee, Knoxville, Tennessee 37996-1200}

\textsuperscript{2}Solid State Division, Oak Ridge National Laboratory 
\textit{Oak Ridge, Tennessee 37831}

\textsuperscript{3}Physics Division, Oak Ridge National Laboratory 
\textit{Oak Ridge, Tennessee 37831}

Abstract

We present a new quantum Monte Carlo algorithm suitable for generically complex problems, such as systems coupled to external magnetic fields or anyons in two spatial dimensions. We find that the choice of gauge plays a nontrivial role, and can be used to reduce statistical noise in the simulation. Furthermore, it is found that noise can be greatly reduced by approximate cancellations between the phases of the (gauge dependent) statistical flux and the external magnetic flux.

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In quantum mechanics, although the Schrödinger equation is complex, in many situations it can be studied in a real representation. Such a representation can often greatly simplify our analysis for those quantum systems. However, there are some problems in which the complexity is unavoidable, in the sense that such problems cannot be made real through a gauge transformation. Examples of such generically complex problems are systems with external magnetic fields or, in two dimensions, systems of anyons.

Previous numerical investigations using quantum Monte Carlo (QMC) methods have been mainly restricted to ‘real’ systems. In this paper, we introduce a QMC method appropriate for the simulation of these generically ‘complex’ systems. Although our approach is quite general, we will illustrate our method on a two dimensional square lattice system. In 2D, it is well known that quantum particles may be anyons of arbitrary statistics, which is defined by the phase $\theta$ of the wavefunction obtained upon interchanging two identical particles. Anyons can be represented as hard-core bosons with appropriate (fictitious) attached flux tubes [1]. In this representation, a fermion is a boson with precisely one flux quantum attached, whereas no flux is attached to a boson. It is clear that either the statistical flux in the anyon systems, or the magnetic flux when there is an external field, gives rise to systems which are intrinsically complex.

For QMC simulations to be practical, it is important to achieve a well controlled noise to signal ratio within a reasonable computer simulation time. For this reason, the application of MC techniques to fermionic systems at low temperature has been largely infeasible due to the infamous ‘sign’ problem [2]. In complex problems, or in the complex representation of the real problems that we will describe below, there is a more general ‘phase problem’ which can lead to equally devastating effects on the simulations [3]. However, our choice of two-dimensional problems allows us to explore a continuum of possibilities between the well-controlled boson problem and the relatively intractable problem of many fermions. Also, since it is as easy to incorporate magnetic fields as fractional statistics, this algorithm makes it possible to explore the interplay between the two kinds of flux [4].

Our method is an unbiased form of the diffusion MC algorithm [5]. For illustration we
consider a tight-binding Hamiltonian of spinless particles on a 2D lattice $H = H^0 + H^1$
where
\[
H^0 = -t \sum_{\langle i,j \rangle} (e^{i\phi_{ij}} b_i^+ b_j + H.c)
\]  
(1)
is the hopping term with $i, j$ representing site indices, and $H^1 = H^1(\{n_i\})$ contains interactions as well as possible couplings to some external scalar potential. In the above expression, we use a second quantized notation in which $b_i^+, b_j$ are bosonic creation and annihilation operators, subject to the hard-core constraint so that the site occupation number operator $n_j = b_j^+ b_j$ has eigenvalue zero or one. $\phi_{ij}$ is the phase associated with the hopping, which may have contributions from the statistical flux as well as from the external magnetic flux. The Schrödinger equation of this system can be mapped onto a diffusion problem by performing a Wick rotation $t \rightarrow -i\hbar\tau$, resulting a diffusion equation
\[
-\frac{\partial}{\partial \tau} |\psi(\tau)\rangle = H |\psi(\tau)\rangle ,
\]  
(2)
which can be simulated through an algorithm of weighted random walks [3]. Generalizations to the continuum or to particles with spin are straightforward. Consider the wave function $Q(Z, \tau) \equiv \langle Z | \psi(\tau) \rangle$, where $\{|Z\rangle\}$, in which $H^1$ is diagonal, spans the Hilbert space of a system with a fixed number of particles $N_p$. The discretized time evolution of $Q(Z, \tau)$ is given by
\[
Q(Z, \tau + h\tau) = W_{diag}(Z; \tau, \tau + h\tau) \sum_{Z'} h_{\tau} r_{Z'\rightarrow Z} W_{transition}(Z', Z; \tau, \tau + h\tau) Q(Z', \tau) ,
\]  
(3)
where the diagonal weight $W_{diag}$ and the off-diagonal weight $W_{transition}$ are given by
\[
W_{diag}(Z; \tau, \tau + h\tau) = \exp\{-V(Z, \tau) - \sum_{Z' \neq Z} r_{Z' \rightarrow Z} h_{\tau}\} ,
\]  
(4)
\[
V(Z, \tau) = \langle Z | H^1 | Z \rangle ,
\]  
(5)
and
\[
W_{transition}(Z', Z; \tau, \tau + h\tau) = e^{i\phi_{ij}} .
\]  
(6)
One can verify that equation (3) indeed reduces to the diffusion equation in the limit of $h_\tau \to 0$. The quantity $r_{Z' \to Z}$ can be interpreted as the transition rate from state $|Z'\rangle$ to the state $|Z\rangle$ due to $H^0$, so that the probability $p_{Z' \to Z}$ for such a transition taking place during time $h_\tau$ is $h_\tau r_{Z' \to Z}$. Thus, starting with an initial state, one can generate random walks according to $p_{Z' \to Z}$, and compute the corresponding weight factors. The diagonal weights $W_{\text{diag}}$ contain two factors, representing the external scalar potential $V$ and the kinetic energy. The off-diagonal weights $W_{\text{transition}}$ are always a pure phase, with $\phi_{ij} = \int_i^j \vec{A} \cdot d\ell$ arising from a vector potential $\vec{A}$ which represents the statistical and/or external flux.

We now consider the calculation of physical observables at zero temperature, in particular the ground state energy $E_0$. As $\tau \to \infty$, one has

$$|\psi(\tau)\rangle = e^{-E_0\tau}|\psi_0\rangle\langle\psi_0|\psi(\tau = 0)\rangle + \mathcal{O}(e^{-(E_1-E_0)\tau}) ,$$

where $|\psi_0\rangle$ is the ground state of the system and $E_1$ is the next lowest eigenvalue of $H$. The ground state energy can be calculated from (7) through, e.g., the logarithmic derivative of $\langle\psi(\tau)|\psi(\tau)\rangle$. Actually, it is not necessary to compute $|\psi(\tau)\rangle$ explicitly, since the ground state energy can be determined directly from the weight functions (4) and (6). To see this, note that the ground state energy $E_0$ may be extracted equally well by multiplying to (7) any state $|x\rangle$ not orthogonal to $|\psi_0\rangle$. If we take $|x\rangle = \sum_Z |Z\rangle [5]$, we have

$$E_0 = \lim_{\tau \to \infty} \frac{1}{\Delta \tau} \ln \{ \sum_Z Q(Z, \tau)/ \sum_Z Q(Z, \tau + \Delta \tau) \}$$

$$= \lim_{\tau \to \infty} \frac{1}{\Delta \tau} \ln \{ \sum_{i=1}^{N_{\text{rw}}} W_{\text{tot}}^i(Z; 0, \tau)/ \sum_{i=1}^{N_{\text{rw}}} W_{\text{tot}}^i(Z; 0, \tau + \Delta \tau) \} .$$

(8)

where $N_{\text{rw}}$ is the total number of random walks generated in the simulation, and the total weight function $W_{\text{tot}} \equiv W_{\text{diag}}W_{\text{transition}}$. In our actual simulations discussed below, the random walks generated by $p_{Z' \to Z}$ are sampled using the usual single move Metropolis method. $E_0$ is computed through (8) as the mean of a large sample of random walks, while the statistical fluctuations of such a sampling are measured from its variance. To illustrate the algorithm and for the purpose of investigating the effect of the ‘complexity’, we have not guided the random walks or done any other importance sampling. For sufficiently small time
step \( h_{\tau} \), the systematic error comes from the finite simulation time \( \tau \) being used during an actual simulation. The statistical noise, as we show below, depends strongly on the strength of the two sources of phase (the two fluxes) in the problem. It also in general increases rapidly with increasing \( \tau \) as \( \tau \to \infty \). Hence an accurate result for zero temperature often requires a choice of finite \( \tau \) which gives the best compromise between the decreasing systematic error and the increasing sampling error. As an example, we show in Fig.1 the MC result for three particles with various statistics on a \( 4 \times 4 \) lattice with free boundaries. We see that the noise increases with statistics approaching the fermion limit. For this system there is a level crossing, near \( \theta = 0.6 \), at which the ground state changes its symmetry. In this case, one needs to multiply some additional symmetry breaking factors to the weight \( W_{\text{tot}}^i \) in (8) to ensure extracting the correct ground state properties; in the absence of such a correction, our algorithm tracks the excited state of the appropriate symmetry (as shown). The calculation illustrated in Fig.1 is, to our knowledge, the first QMC simulation for anyons.

It is clear that any physical observable computed should be independent of the choice of the gauge. However, it is less obvious that the statistical fluctuations associated with the QMC simulations described above might not in fact be quite sensitive to the gauge adopted. To illustrate the effect of gauge choice on statistical fluctuations, let us consider the ‘string gauge’ [7]. One may, for example, attach a single string to each bare boson so that there is a phase factor \( e^{\pm i\theta} \) multiplying the off-diagonal weight whenever a particle crosses a string (or vice versa). (Since the strings have to end somewhere, it is a nontrivial task to construct a gauge theory for finite systems which are self-closed (such as a torus). In the following we shall restrict ourselves to problems with open boundary conditions where such complications are not present.) For bosons, all weights are positive, and no cancellation occurs. As the statistical angle \( \theta \) is tuned away from zero, \( W_{\text{tot}}(Z; 0, \tau) \) becomes complex. In general we expect that the sum of the \( W_{\text{tot}}^i \) in (8) is also a complex number with a phase \( \phi_m \). One can study fluctuations by considering an additional time increment \( h_{\tau} \) after some (long) time \( \tau \). In this gauge the phase gained by a single MC move can have \( 2N_p - 1 \) values, and has an angular variation of amplitude \( (2N_p - 1)\theta \). Here we see that phase fluctuations are
minimized in the small $\theta$ and/or small particle number limit. For fermions ($\theta = \pi$), we have a situation where the off-diagonal weights are real and fluctuate between the positive and negative part of the real axis, commonly known as the ‘sign problem’.

Now consider the gauge of $M$ strings per particle. On a finite square lattice, the maximum number of strings that can be attached to a particle is $4L$, where $L$ is the linear size of the lattice. Each string can share a statistical phase $\theta/M$. Depending on how closely two particles are placed, the phase acquired from a single hop of one particle can be as large as $\theta/4$, or as small as $\theta/M$ (assume $M \geq 4$). Considering the dilute limit (in which the lattice approaches a continuum) where the probability for two particles coming close to each other is negligible, the average phase fluctuation caused by an additional MC move after time $\tau$ is of order $(2N_p - 1)\theta/M$. For $M = 4L$, we see that for a given $\theta$, the average phase fluctuation is reduced by a factor of the order of the system size.

The simple argument given above should be treated with some caution. However, our argument does suggest, in an intuitive way, that fluctuations can be reduced considerably by spatially ‘spreading’ the gauge. (We note that there is some support for this conclusion, in a different context, in Ref. [7].) Thus, from this point of view, it is quite plausible that the optimum choice of the gauge which minimizes the statistical fluctuations with a given number of random walks would be the continuous gauge (CG) $[A_\phi = (\theta/\pi r)\hat{\phi}]$ which simply uses the azimuthal increment $\delta\phi$ to determine the phase increment associated with a hop. In this gauge the change of phase associated with each MC move is minimum on average. Furthermore, this argument suggests that the CG will be most useful in the dilute limit, in which the angular (and hence phase) increments can be made very small on average. (Of course, in this limit, any method will find some relief from statistical noise since the effect of statistics—e.g., the Fermi energy—is vanishing, regardless of gauge.) We have carried out various simulations, using the diffusion algorithm described above for free, spinless particles in 2D to test the above conjecture. In Fig.2 we show a comparison of the single-string (1S) gauge and the CG, for six spinless fermions on a 20x20 lattice (filling 0.015). The CG estimate is seen to be converging smoothly (although slowly, due to the small excitation
gap) to the exact result (calculated independently) with increasing $\tau$, with bounded error estimates for $\tau < 4.5$, while the 1S results give unbounded error in the same range of $\tau$. We obtain this bound by examining the variance of the distribution of (complex) weights to see if it scales as $1/\sqrt{N_{rw}}$. This is essential since even extremely noisy samplings can give—on occasion—a relatively small sample variance. Points which fail to meet this scaling criterion (and hence have a sample variance which is not statistically reliable) are marked with parentheses in Figs. 2 and 3; the improvement obtainable by using the CG is evident.

Now we explore the interplay between the statistical flux and external flux. As discussed previously, the presence of external flux may lead to large noise in QMC simulations, just as the statistical flux can [3]. However, with the presence of both fluxes, we have found that there is a nontrivial cancellation between the two, resulting significant improvement in the signal to noise ratio in QMC simulations. Fig.3 shows results for the simulation of 4 fermions (treated in the CG) on a $4 \times 4$ lattice with an external magnetic field. Without the field, the statistical noise is unbounded (by our previous criterion) within the given computational time; as the external field is increased (with the gauge choice such that the statistical flux opposes to the external one), noise is reduced progressively, such that, in the same simulation time, the energy estimate converges to the exact result with much smaller statistical error. Presumably the convergence rate is enhanced by the larger gap in the case with flux; however, it is clear from the figure that it is the statistical noise itself, arising from the large phase fluctuations in the zero-field case, which renders the simulation unmanageable. Finally, we note that increasing the field beyond the optimal value again increases the statistical noise, so that it resembles the simulation shown in Fig.3 for the zero-field case.

To summarize our results, we have introduced a new QMC technique for simulations of generically complex problems. Using a complex (anyonic) representation of the many fermion system (which is not possible for QMC in its real form), we find that statistical fluctuations can be significantly reduced by an appropriate choice of gauge. This method is presumably most effective in dilute systems in which the average phase change in a single
MC move is small. Furthermore, we find that there exist nontrivial cancellations between statistical flux and external flux for some external fields, resulting in considerable reduction of the statistical error. This may be utilized in QMC simulations for these systems.

There are some works in the literature exploring ‘complexity’ in QMC simulations [8], most notably references [9] and [10]. We would like to remark that our algorithm is a general formalism which contains the problems studied in these works as special cases, and which allows one to simulate more general systems, such as anyons (or fermions in the anyonic representation). Furthermore, unlike the QMC methods commonly employed for lattice problems which utilize the Hubbard-Stratonovich transformation, this algorithm requires no prior knowledge of single particle states. This has thus the advantage that it permits one to simulate problems for which such knowledge does not exist or is difficult to compute (such as anyons). Finally, we note that our method requires small memory space on a computer so that it is readily parallelized.

In closing, we wish to mention some physical problems which might be investigated within this algorithm. First, it is clear that our conclusions for fermions hold for anyons in general. The anyon problem is of some physical interest both for its (possible) superconductivity properties and for its relevance in the fractional quantum Hall effect [1]. This algorithm, possibly enhanced by importance sampling in the generation of random walks, should allow the study of anyon systems with sizes not accessible to exact diagonalization. We have also shown that representing fermions with a complex ‘anyon’ gauge can reduce the sampling noise. This reduction is however most pronounced for dilute fermions, where other methods are already successful. Hence we believe that a reformulation of the problem in the continuum (rather than on a lattice) should be explored, since this case the continuous gauge will have greatest efficacy over the usual single-string gauge. Application of our method to a continuum involves greater computational demands but presents no conceptual difficulties.

Another problem involving external flux is the question of flux quantization [10][11], as measured by the dependence of the ground-state energy upon a localized external flux. We
have already tested our method on the (hard-core) boson case, on lattices up to $10 \times 10$ in extent at $1/4$-filling. Interesting physical applications arise on extending the method to bosons with disorder [12], or to anyons [13]; in principle, fermions [10] can also be studied with this method as well. Finally, electrons in two dimensions in a magnetic field is a problem of great current interest. Our approach promises to be most useful at filling fractions which give a commensuration of particles to flux, i.e., the quantized Hall effect (QHE). It should be straightforward to test for signs (such as a cusp in the energy) of a QHE, for fermions or anyons on a continuum, or for particles on a lattice [13].

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FIGURES

Figure 1. Energy $E_0$ vs. statistics angle $\theta/\pi$, estimated using the continuous gauge for the statistical ‘flux’. The continuous lines give exact eigenvalues, obtained by Lanczos diagonalization. Sampling variance is indicated by error bars. We see that, by appropriate choice of weighting of the random walks, our algorithm can select either the ground state or the lowest excited state of a different symmetry.

Figure 2. Ground-state energy estimate for 6 fermions on a 20x20 lattice, as a function of the time $\tau$, with fixed sample size ($= 4 \times 10^6$ walks). The horizontal line marks the exact energy. For clarity, the 1S results are displaced upwards by +5. Some points are marked with parentheses to indicate that the computed variance is not statistically reliable.

Figure 3. Ground-state energy estimate for 4 fermions on a 4x4 lattice, as a function of $\tau$; sample size is $16 \times 10^6$ walks. Again, the horizontal line gives the exact result. The zero field case is displaced by +5.