

Model fermion Monte Carlo with correlated pairs

M.H. Kalos

Center for Theory and Simulation in Science and Engineering

and

Laboratory of Atomic and Solid State Physics

Cornell University

Ithaca, New York 14853

Abstract

The issues that prevent the development of efficient and stable algorithms for fermion Monte Carlo in continuum systems are reexamined with special reference to the implications of the “plus/minus” symmetry. This is a property of many algorithms that use signed walkers, namely that the dynamics are unchanged when the signs of the walkers are interchanged. Algorithms that obey this symmetry cannot exhibit the necessary stability. Specifically, estimates of the overlap with any antisymmetric test function cannot be bounded away from zero in the limit of many iterations. Within the framework of a diffusion Monte Carlo treatment of the Schroedinger equation, it is shown that this symmetry is easily broken for pairs of walkers while at the same time preserving the correct marginal dynamics for each member of the pair. The key is to create different classes of correlations between members of pairs and to use (at least) two distinct correlations for a pair and for the same pair with signs exchanged. The ideas are applied successfully for a class of simple model problems in two dimensions.

1. Introduction

This paper continues a discussion of possible Monte Carlo algorithms intended to solve the non-relativistic Schroedinger equation for fermions in continuous space. In particular, it succeeds the paper of Liu, Zhang, and Kalos [1] (LZK); see also references therein.

We take the opportunity here to sketch the basic issues in a very general way. Wave

functions are represented by ensembles of points in the configuration space required for the physics of the problem. Each such point usually contains cartesian coordinates for all of the interacting particles. Since those coordinates change following stochastic dynamics appropriate for the mathematical problem, it is reasonable to think of them as random walkers in configuration space. For an N -body system in three dimensions $R = \{x_1, y_1, z_1, x_2, \dots, y_N, z_N\}$. More generally, we may deal with ensembles of such walkers, $\mathbf{R} = \{R_1, R_2, \dots, R_K\}$. In either case, we will introduce stochastic dynamics that produce random walks for R or for \mathbf{R} . On the average, the density of walkers $\chi^{(n)}(R)$ at the n -th stage of such a walk for R satisfies

$$\chi^{(n)}(R) = \lambda \int g(R, R') \chi^{(n-1)}(R') dR' \quad (1)$$

or the global density of the entire population satisfies

$$X^{(n)}(\mathbf{R}) = \Lambda \int G(\mathbf{R}, \mathbf{R}') X^{(n-1)}(\mathbf{R}') d\mathbf{R}' \quad (2)$$

As with all Monte Carlo calculations, a solution of the equations is represented as a sum of delta functions:

$$\psi(R) \cong \sum \delta(R - R_m) \quad (3)$$

where $\{R_m\}$ is the set of positions attained by a random walker, possibly after some initial equilibration. The dynamics must be such that

$$\lim_{n \rightarrow \infty} \chi^{(n)}(R) = \psi(R) \quad (4)$$

where $\psi(R)$ is a solution of the Schroedinger equation.

In general, we will use some test function $\phi_T(R)$ to project the walker positions so as to obtain integrals of solutions of the Schroedinger equation. For fermion systems, ϕ_T must be an appropriately antisymmetric function $\phi_{AT}(R)$. To solve a fermion problem within this framework, the dynamics must be such that

$$\lim_{n \rightarrow \infty} \int \chi^{(n)}(R) \phi_{AT}(R) dR = C \int \psi_A(R) \phi_{AT}(R) dR \quad (5)$$

where $\psi_A(R)$ is an antisymmetric solution of the Schroedinger equation and C is a non-zero constant independent of ϕ_{AT} .

Multiplying the Schroedinger equation:

$$H\psi_A(R) = E_A\psi_A(R) \quad (6)$$

by $\phi_{AT}(R)$, integrating over all coordinates, and using the hermiticity of H , one obtains

$$\begin{aligned} E_A &= \frac{\int \psi_A(R) H \phi_{AT}(R) dR}{\int \psi_A(R) \phi_{AT}(R) dR} = \frac{\lim_{n \rightarrow \infty} \int \chi^{(n)}(R) H \phi_{AT}(R) dR}{\lim_{n \rightarrow \infty} \int \chi^{(n)}(R) \phi_{AT}(R) dR} \\ &= \frac{\sum_m H \phi_{AT}(R_m)}{\sum_m \phi_{AT}(R_m)} \end{aligned} \quad (7)$$

Collective dynamics, if used, must produce distributions $X^{(n)}(R)$ of ensemble positions such that

$$\lim_{n \rightarrow \infty} \int \cdots \int X^{(n)}(\mathbf{R}) \phi_{AT}(R_j) dR_1 \cdots dR_k = C' \int \psi_A(R) \phi_{AT}(R) dR$$

for every j . That is, the marginal distribution for every R_j must project to ψ_A in this way.

It is by now well known that the ordinary dynamics– Green’s function Monte Carlo or diffusion Monte Carlo, have symmetric functions as their asymptotic distributions. Thus the integrals in both numerator and denominator of Eq. (7) have zero as their limits. We will not review here all of the various methods that have been invoked to overcome this essential difficulty. Instead, we concentrate on the general ideas following Arnow et al. [2], Zhang and Kalos[4] (ZK), and LZK.

We consider some form of collective dynamics involving random walkers, equal numbers of which carry positive and negative signs. The dynamics are “collective” in the sense that all or many members of the ensemble determine the future stochastic behavior of any

member. The different signs help to represent the antisymmetric wave function (which is not everywhere positive) and also offer the possibility that cancellation can occur between walkers of different signs, and that the resulting population will be such that the integrals that appear in equation (7) will be asymptotically different from zero. We call dynamics that produce such a result “asymptotically stable.” If one is willing to let the population of walkers grow exponentially, with a sufficiently large coefficient, then asymptotic stability is easy to attain. The penalty is that the variance decreases only as the inverse of the logarithm of the computing time rather than as its inverse.

In several papers, ZK introduced the notion of the “plus/minus” symmetry, a way of considering whether some proposed collective dynamics might be asymptotically stable. The criterion is simple: suppose that at a certain stage of a collective dynamics, the configuration R consists of equal numbers of positive walkers: $\{R_k^+\}$ and of negative walkers $\{R_k^-\}$. Suppose also that one interchanges the two subpopulations

$$R_k^+ \rightarrow R_k^-; R_k^- \rightarrow R_k^+ \quad (8)$$

for every k . If the dynamics cannot distinguish between the original collective configuration and the interchanged configuration, then both will be represented equally in the asymptotic population. In that case, the integrals in Eq (7) will again be zero. Therefore, a necessary condition for stability is that the dynamics breaks the plus/minus symmetry.

The collective dynamics of the kind introduced by Arnow et al. [2] clearly do not break this symmetry. Although ZK believed that their introduction of a collective importance sampling had that effect, it is not so: importance sampling cannot break the symmetry when the original dynamics have not done so. This applies also to the versions of the dynamics of Arnow et al. that have been used by Anderson and his coworkers[3]. Although these forms of collective dynamics are very likely to slow down the decay to the symmetric distribution, they cannot entirely stop it. Also, the issue remains of the scaling to large systems. These forms of collective dynamics involve large ensembles of interacting walkers,

and although the scaling has not been studied experimentally, it is plausible that as the system size grows, the size of the interacting ensemble will have to be made larger. Since the complexity of the method appears to grow with the square of the ensemble size, it is not obviously promising.

LZK, for the first time, exhibited an exact method using at most pairs of walkers for the Monte Carlo integration of the Schroedinger equation so as to yield solutions antisymmetric in the origin. Although the method applied to highly artificial model problems— particles in various enclosures with no potentials, or else with potentials satisfying certain artificial inequalities— it is a provocative result, one that we will summarize here. Direct reference to the paper would be very helpful.

Consider a two-dimensional enclosure (such as a parallelogram) in which a solution to the Schroedinger equation that is antisymmetric on reflection in the origin is required. Divide the enclosure into four subregions by two orthogonal straight lines. Walkers are started in one of these four subregions (either one that contains both of the reflections of two of the other subregions in the lines.) Walkers that cross either of the two lines for the first time are turned into two of opposite sign (each with a weight of one half) where the new point is the reflection in the origin of the original. The paths of the two walkers are thereafter constrained to be reflections on the line first touched. The first passage across the orthogonal line— which occurs with probability one— is guaranteed to be at the same point. Two walkers of opposite sign that arrive at the same point cancel each other and can be dropped from consideration.

The essential features of LZK, which seem important to retain, are the following: The dynamics couples a positive and a negative walker using two distinct correlations in such a way that the marginal dynamics for each walker is correct. Cancellation between plus and minus walkers is possible. The outcome is that the symmetry is broken by a geometric construction, not dependent on unknown features of the solution, such as the nodal surface.

The generalization of LZK to problems with arbitrary potentials in many dimensions

is not at all obvious. This paper is devoted to one possible extension. Since the motivation is easiest to give, and the applications carried out lie with the framework of simple diffusion Monte Carlo, we first devote a short section to an exposition of the algorithmic character of importance-sampled diffusion Monte Carlo for the Schroedinger equation.

2. Diffusion Monte Carlo

Following the general structure of Green's function Monte Carlo, Ceperley [5] showed that with the use of a finite time step, δ , the Schroedinger equation in imaginary time, modified by an importance sampling transformation, can be integrated by a particularly simple Monte Carlo procedure. We do not propose to repeat the derivation here nor any extensive discussion; they are well known. Rather, we need simply to recall its essence.

Consider a hamiltonian $H = -\frac{1}{2}\nabla^2 + V(R)$. Ceperley derives the evolution of the Schroedinger equation in imaginary time τ from the operation of $\exp[-\tau(H - E_T)]$ upon some initial function $\psi(R, 0)$:

$$\psi(R, \tau) = \exp[-\tau(H - E_T)]\psi(R, 0) \quad (9)$$

E_T is a number that approximates to the lowest eigenvalue. Let $\phi_T(R)$ be some trial function that approximates to the ground state solution, $\psi_0(R)$, and

$$f(R, \tau) = \phi_T(R)\psi(R, \tau) \exp(E_T\tau) \quad (10)$$

Then a random walk, that consists of three steps in turn, will generate a population of walkers whose density is $f(R, \tau)$. If the method is iterated long enough,

$$f(R, \tau) = \phi_T(R)\psi_0(R) \exp[(E_T - E_0)\tau] \quad (11)$$

from which estimates of the eigenvalue and other information that relates to the solution $\psi_0(R)$ may be derived.

The three steps that take a walker at position R_m and imaginary time τ into a position R_{m+1} at time $\tau + \delta$

(1) Drift: a displacement by the many-dimensional vector

$$\delta \vec{\nabla} \phi_T(R_m) / \phi_T(R_m) \quad (12)$$

(2) Diffusion: a displacement by the $3 - N$ dimensional random vector $\sqrt{\delta} \vec{U}$, where each component of \vec{U} is a Gaussian random variable with mean zero and variance one.

The outcome of steps (1) and (2) is that the walker is moved to

$$R_{m+1} = R_m + \delta \vec{\nabla} \phi_T(R_m) / \phi_T(R_m) + \sqrt{\delta} \vec{U} \quad (13)$$

(3) Branching: After the diffusion step, each walker is replaced by a random number of identical walkers, the average number now being

$$\exp\{-\delta[H\phi_T(R_{m+1})/\phi_T(R_{m+1}) - E_T]\} \quad (14)$$

In particular, if $\phi_T(R)$ were an eigenfunction and

$$H\phi_T(R) / \phi_T(R) = E_T \quad (15)$$

then there would be no branching at all: a walker lives forever.

3. Correlated pairs of plus/minus walkers

We are now in a position to consider how to introduce correlated walks of pairs of walkers that carry opposite signs, guided by the principles derived from LZK.

If the Monte Carlo is indeed to involve pairs, (R_m^+, R_m^-) that live forever or for a long time, then there should be little branching of the two independent of each other. One way to assure this is to use the symmetric ground state as an importance function. We shall assume it known for the moment. In fact we will construct model problems starting from an assumed ground state, $\psi_0(R)$. Furthermore we will set

$$E_T = H\psi_0(R) / \psi_0(R) \quad (16)$$

To assure correct marginal dynamics, we simply apply to each of the walkers (R_m^+, R_m^-) the three steps outlined in the previous section.

One simple class of correlations between the two walkers relates the Gaussian vectors (U^+, U^-) that are used in the diffusion steps for (R_m^+, R_m^-) respectively. Note that the same Gaussian distribution is to be sampled at every diffusion step. Thus we can correlate the U^+ with U^- in many ways that are technically easy to achieve. For example, putting $U^+ = U^-$ or $U^+ = -U^-$ achieves a potentially useful kind of correlation between the positive and the negative walkers, while trivially preserving the correct marginal dynamics. We call these “parallel” correlation dynamics and “antiparallel” correlation dynamics respectively.

Within that basic class of correlations, there are clearly many ways of relating the Gaussian vectors (U^+, U^-) . We introduce one more as of particular interest. Suppose that the positions of the two walkers just after each has been moved by a “drift” step are R_m^+ and R_m^- respectively. Construct the hyperplane that is the perpendicular bisector of the line from R_m^+ to R_m^- . Now let U^- be the reflection of U^+ in that hyperplane. What is special about this relation of the vectors is that the relative distance $|R_m^+ - R_m^-|$ of successive positions is a one-dimensional variable that undergoes a random walk, which, with probability one, brings the pair eventually to positions where $R_m^+ = R_m^-$. In other words, this “reflected” correlation dynamics guarantees eventual cancellation of the pair (R_m^+, R_m^-) . This cancellation will be efficient even in many dimensions. It can be accelerated by sampling pairs (R_m^+, R_m^-) from the kernel constructed from the difference of the Green’s functions centered at R_m^+ and R_m^- respectively, enforcing the reflection symmetry in the new values of R_m^+ and R_m^- .

We are now in a position to ask which of the three kinds of correlation dynamics is most promising for a fermion algorithm based on diffusion Monte Carlo. Since we have stressed the need for cancellation of pairs, and since the third kind, reflected correlation dynamics, satisfies that requirement, it would seem to be the optimal choice. But that is not correct. In fact, none of the choices mentioned so far, or other possible choices of

this kind, by themselves, will lead to a stable fermion method. The reason is easily stated: their dynamics do not break the “plus/minus” symmetry. Consider, for example, reflection dynamics applied to two pairs in which $R_m^+ = R_1, R_m^- = R_2$ and $R_m^+ = R_2, R_m^- = R_1$ respectively. The bisecting hyperplane is the same in both cases; the dynamics for both are exactly the same. The same argument holds, pair by pair, for all of an ensemble of pairs. Thus the dynamics do not make the necessary distinction between these pairs.

A solution is one step beyond what has been done: If we use *dynamics correlated in different ways* for the two interchanged pairs given above, then the symmetry is broken in a very simple way. This, then, is the key to a stable fermion algorithm.

How, then might such an algorithm be constructed? We need at least two different kinds of correlated dynamics, and we need some rules for when to apply each kind. At the moment, we have neither experience nor theory of how to choose the dynamics and the rules in optimal or at least clearly intelligent ways. We proceed heuristically.

First, entirely for simplicity, we limit consideration to just two classes of dynamics. In order to have cancellation, reflected correlation dynamics is one of them. Parallel correlation offers the possibility of preventing cancellation of pairs whose configuration is favorable, so we choose it as the other kind.

Rough criteria for the rules of application follow from these arguments: we will use reflected dynamics for pairs not likely to make a long term contribution to the overlap with a particular antisymmetric test function ϕ_{AT} , and parallel dynamics for pairs likely to make such a contribution. We will describe our choices in more detail in the context of the test problems given below.

4. Model Problems

For simplicity and to aid in visualization of results, we have chosen to address the Schroedinger equation in two dimensions. We must consider problems for which the ground state is symmetric on reflection in the origin. As indicated at the beginning of the previous section, it is technically useful to treat problems whose ground states are known explicitly.

To create a variety of test problems, one can simply write down the ground state wave function as

$$\psi_0(r) = \sum_k \exp[-\frac{1}{2}(r - r_k)^2] \quad (17)$$

where the r_k are arbitrary positions in two dimensions. To assure invariance on reflection in the origin, the r_k occur in pairs, say r_k and r_{-k} with $r_{-k} = -r_k$.

The potential that gives that eigenfunction and an eigenvalue of unity is

$$V_0(r) = \frac{\sum_k (r - r_k)^2 \exp[-\frac{1}{2}(r - r_k)^2]}{2 \sum_k \exp[-\frac{1}{2}(r - r_k)^2]} \quad (18)$$

This potential can, by various choices of the set $\{r_k\}$, be either well structured or not. A well structured potential is characterized by the the symmetries it has, in addition to the required symmetry of invariance in reflection in the origin.

5. A Model Computer Program

An unsophisticated Monte Carlo program was written to test whether the scheme outlined above does indeed break the plus/minus symmetry in a stable way and does give correct distributions and eigenvalues for antisymmetric solutions of the model problems described.

To avoid the complexities of managing the full range of population fluctuation, the program uses a fixed number of pairs M , given as input. More specifically, a pair is selected at random from the population, and advanced one time step. The move may, of course result in cancellation; the process is repeated until a new population of size M is developed. This introduces a bias of order $1/M$ in results derived from the calculations. As we shall see, that bias combined with one resulting from the fixed time step, δ , appears to produce a somewhat complicated source of numerical error.

The code has various options for selecting pairs of r_k , the potential centers defined in Eq. (18). One member of a pair may be chosen from a Gaussian distribution with specified

variance; the other is obtained by reflecting in the origin. Alternatively, values may simply be read in. Potentials that are more or less well structured may be specified in this way. A limiting case is a pair of centers at the origin, which gives the standard two-dimensional harmonic oscillator.

The program allows three regimes in the time evolution, each may have a different time step δ . Walkers are followed for different numbers of time steps in each of these regimes; data for eigenvalues and for histograms of the distributions are accumulated only in the last. In practice, δ was set large in the first stage to allow a coarse-grained relaxation to the equilibrium distribution; in the intermediate regime, a value of δ was used within a factor of two of that in the last.

The test function, $\phi_{AT}(x, y)$, was chosen to be the anisotropic harmonic oscillator

$$\phi_{AT}(x, y) = y \exp[-a_1^2 x^2 - a_2^2 y^2] \quad (19)$$

rotated through an angle set to be θ_T . Values of a_1 , a_2 , and θ_T were determined by rough variational minimization; some values of θ_T were found by maximizing the integral in the denominator of Eq. (7) with respect to θ_T during preliminary runs.

The program provides two alternative forms for creating an initial population of pairs: In one, M points are sampled from Eq. (19) and assigned as coordinates of positive walkers. Negative walkers are obtained by reflecting in the x -axis; then both members of the pair are rotated through the angle θ_T . The second possible initialization requires input values for all four coordinates of the pair. In any case, the code generates correlated pairs of positive and negative walkers: each member of a pair follows the drift appropriate for its position as determined from the ground state wave function given by Eq. (17) and the set $\{r_k\}$. The Gaussian steps of the two walkers are correlated: if the Gaussian in two dimensions appropriate for one of the walkers is \vec{u} , then the other is either \vec{u} (“parallel” or “p-correlated” dynamics) or it is the vector \vec{u} reflected in the bisector of the line from one walker to the other (after the drift is carried out.) for “reflected” (or “r-correlated”)

dynamics.

An important element of the proposed method is the criterion for choosing between p-correlated and r-correlated dynamics. As has been indicated, there is not yet any theory or experience for doing this. In the experimental program, it was done as follows: Let $\vec{\omega}_0$ be a unit vector and r_0 a length both of which are specified as input. Then a pair, $\{\vec{r}^+, \vec{r}^-\}$ will use p-correlated dynamics if both

$$\vec{\omega}_0 \cdot (\vec{r}^+ - \vec{r}^-) > 0 \tag{20a}$$

$$(\vec{r}^+ - \vec{r}^-)^2 > r_0^2 \tag{20b}$$

and r-correlated dynamics otherwise.

A little experimentation showed that the overlap in the denominator of Eq. (7) depends on the orientation of $\vec{\omega}_0$. Generally speaking, one expects $\vec{\omega}_0$ to point from the regime in which ψ_A , the antisymmetric solution, is negative to the region in which it is positive. All orientations gave stability, however. There has as yet been no attempt to study the sensitivity to values of r_0 .

A second program was written to solve the same Schroedinger equation by a simple relaxation method on a two dimensional mesh of spacing h . The solution was assumed to vanish beyond a distance cutoff. Explicit antisymmetrization of the solution was carried out after every relaxation pass through the mesh. The eigenvalue was computed by trapezoidal integration for the numerator and denominator of Eq. (7). Experiment showed that the error of the eigenvalue was proportional to h^2 . In addition the cutoff was varied to correct for the numerical error that it introduces.

6. Results

6.1 Simple harmonic oscillator

Since the model program has, as a special case, the simple harmonic oscillator, it is useful to run that case as a check on both Monte Carlo and relaxation programs.

The results of four runs of the finite difference program are shown in Table I. As will be seen, the mesh spacing was varied for constant cutoff and vice-versa. The effect of increasing the cutoff from 5.95 to 6.55 is negligible. The error was studied as a function of h and found to vary as h^2 . On that basis, one may extrapolate to get 2.000004076 for the eigenvalue. The exact eigenvalue is 2. The fact that the extrapolation reduces the error by two orders of magnitude serves to increase confidence in the procedure.

Since the test function $\phi_{AT}(x, y)$ as given by Eq. (19) includes the exact solution for $a_1 = a_2 = \sqrt{\frac{1}{2}}$, an elementary but useful test is to assign those values and run the program; the result was an eigenvalue of 2 (to the numerical precision of the computer.)

More realistic Monte Carlo results are shown in Table II. In these runs, the values $a_1 = a_2 = \frac{6}{10}$, chosen quite arbitrarily, were used. If the population bias is exactly $1/M$, and the time step error is proportional to δ , and the two are independent, then both can be extrapolated from the two sets of results in the tables. The result is an eigenvalue of 1.99883(79), that is, 1.48 standard deviations from the exact result.

In fact, the simple harmonic oscillator is not a serious test of the general methods proposed here. The reason is that the plus/minus symmetry is broken by either one of the dynamics used. The combinations proposed in this paper are not necessary. It is interesting to examine the way in which this works. We start with an ensemble of pairs with a vertical orientation, and with the positive walker about the negative.

As indicated above, the dynamics is controlled by the importance function, which in this case is simply

$$\psi_T(R) = \phi_0(\vec{r}) = \exp(-r^2/2)$$

A drift step then moves from \vec{r} to $\vec{r}(1 - \delta)$. A sequence of drift steps drives a walker toward the origin. For ordinary diffusion Monte Carlo, this is compensated by the diffusion steps that distribute the walkers in a Gaussian centered about the origin.

For a correlated pair of plus/minus walkers, the drift steps act in the same way: A sequence of drift steps drives the center of mass and the relative separation of the pair

towards zero. However, the orientation of the pair– the direction from the negative walker to the positive walkers– is unchanged in such steps.

The effect of parallel-correlated diffusion is as follows: The pair orientation is unaffected; the center of mass is changed by the addition of a Gaussian; and the relative distance is unchanged. An alternation of drift steps and p-correlated steps leaves the direction unchanged, distributes the center of mass in a Gaussian and drives the relative distance to zero.

Steps that use reflection-correlated diffusion with cancellation also preserve the pair orientation . If a pair survives, then the new pair has the same vertical coordinate of the center of mass as the old, but the relative separation changes by a Gaussian. Thus the alternation of drift steps and r-correlated steps leaves the direction unchanged, drives the vertical coordinate of the center of mass to zero, and distributes the relative separation in a Gaussian. Note that r-correlation without cancellation can invert the direction of the pair of walkers.

The outcome of a sequence of drift and correlated steps is that the orientation is preserved. In itself, this breaks the plus/minus symmetry. For example, if the initial population has (as would be natural) a net “polarization” in the sense that the average direction from negative to positive walkers is positive, then that will be preserved. If all initial pairs have the same direction, then that will be conserved. Thus, asymptotically the overlap with a test function will not be equally likely to have positive and negative values.

In fact, if the correlated steps referred to in the last paragraph are always parallel, then the overlap from a pair of walkers will be asymptotically zero, since the separation of the two will go to zero geometrically. However it is possible to show– we will not carry out this here– that an estimator for the eigenvalue can be obtained from these pairs, by including the weight that comes from the factor $\exp[(E_F - E_0)\tau]$.

On the other hand the dynamics that results from using drift and reflection correlation

(with cancellation) applied to an ensemble of pairs correctly solves the simple harmonic oscillator problem and gives asymptotically stable estimates for the integrals needed to determine the eigenvalue.

Finally, we note that if the plus and minus walkers of a pair are initiated as images in a single line, then that relationship is preserved in parallel moves. The outcome of an indefinite sequence of parallel moves is that each member of the pair undergoes random walk that obeys the fixed-node constraint.

The notion, introduced in this paper of using distinct classes of correlated dynamics is therefore not needed for the harmonic oscillator. The problems discussed in the next sections were devised in the expectation that the more or less ill structured potentials would yield drift behavior that would in turn require the use of different dynamics.

6.2 Unstructured problems in two dimensions

In the paper of LZK, a construction was given in which a correlated walk could be extended to Schroedinger equations with potentials provided that special (unphysical) inequalities in the potential were satisfied. Although there is no clear and direct connection between that construction and the algorithm used here, we wanted to avoid satisfying the inequality. Stefan Koch devised a set of potential centers, shown in Table III that are sufficiently unstructured not to obey the inequalities.

The program that solves the Schroedinger equation by finite differences and relaxation gives 1.1467 for the eigenvalue of this problem. A summary of the Monte Carlo results is given in Table IV. The extrapolation to correct for time step and population size biases gives 1.1495 with a standard deviation of 0.0020. The discrepancy between relaxation and Monte Carlo results corresponds to 1.42 standard deviations.

In the Monte Carlo runs, histograms were recorded of the density of positive and negative walkers. The difference of those densities is proportional to the integral of the product of $\phi_{AT}(\vec{r})\psi_A(\vec{r})$ over the two-dimensional bins. By carrying out the same integrations over the same bins using the numerical solution, one can obtain distributions that

can be compared directly with the Monte Carlo. The normalizations are arbitrary so what is required is that ratios of histograms be constant, even when the nodal line is crossed and the signs of both histograms change together. That condition is well satisfied for this calculation and for all the others. The ratios are constant within a few percent except at the edges where the distributions become small.

In the usual analysis of the decay of the signal to noise in the Monte Carlo treatment of fermion problems, the ratio of the eigenvalues for antisymmetric to symmetric solutions plays a key role. Large ratios make the problem worse. In the problem previously discussed, the ratio turned out to be 1.15. In an attempt to find a calculation that is more challenging in that respect, we created another by simply scaling down the positions of the potential centers in Table III by a factor of 0.3 to get the coordinates in Table V. The eigenvalue obtained by numerical relaxation is 1.74753, so that the aim of increasing the eigenvalue towards a value of 2.00 has been achieved. There was no indication of any unstable tendency in the Monte Carlo calculations, so it is not at all clear that shrinking the scale of the potential in this way has posed any additional difficulties. An effect of the rescaling of the potential is to make it smoother, that is to say more like a harmonic oscillator, so that variational estimates based on an anisotropic Gaussian are rather accurate. In that sense, this rescaled potential is not a good test of the generality of the new method.

Table VI gives the results of the Monte Carlo calculations for this problem. In designing this set of calculations, it was assumed that the time step error is proportional to δ and the population bias proportional to $1/M$, and that the two are independent of each other. Thus a run with $\delta = 0.04$ and $N = 500$ can be combined with another having $\delta = 0.02$ and $N = 1000$ by linear extrapolation. The results of this procedure is an eigenvalue of 1.74710 with a standard deviation of 0.00013. The agreement, which appears good, is in fact 3.3 standard deviations. We believe that the explanation lies in the time step and the population errors and in the extrapolation, but have not chosen to pursue the exact elucidation of the errors and their possible interdependence. We believe that the results

do demonstrate the correct solution of the model problem.

In attempt to create one more test calculation that would induce the appearance of instability, Koch devised the set of potential centers shown in Table VII. These extend the range to large distances. The positions of the centers are also shown in Figure 1. The centers are located on two spirals intended to permit positive and negative walkers to drift along different spirals and interchange positions.

In any case, no evidence of an instability in the Monte Carlo calculations was seen in any of many long runs with different program-related parameters. The large extent of the potential does pose difficulties for both numerical relaxation and Monte Carlo: the convergence is slow and more computer time was consumed in assuring reasonable convergence. The eigenvalue obtained from numerical relaxation was 1.018497. Monte Carlo results are shown in Table VIII. Making the same assumptions as before that the population corrections and time step corrections are independent and linear, we extrapolate to an eigenvalue of 1.016748(1124). The discrepancy corresponds to 1.56 standard errors of the Monte Carlo result.

Conclusions

Although the problems actually solved in this study are only two-dimensional, we believe that their correct solution means that the principle introduced in this paper, namely pair dynamics with correct marginal dynamics for each member of a pair and with correlations that vary with the location of the pair does indeed break the plus/minus symmetry and offers the possibility of an accurate and stable solution of fermion Monte Carlo problems in continuum systems.

Clearly much work remains before it can be said that a practical method has been demonstrated that works efficiently on a variety of systems and for large numbers of particles. The method needs to be demonstrated on model and realistic few- and many-body systems in three dimensions.

Many technical issues remain to be explored: When the importance function used

to bias the trajectories are not eigenfunctions, then pairs will occasionally break or else new unpaired walkers will be created. This is not thought to be a major difficulty, but a means for re-pairing walkers needs to be developed. Is it useful to use larger ensembles of correlated walkers than pairs? In more than two dimensions, many more classes of correlations can be invoked. We can only guess whether their use will improve the efficiency and scalability of the method. The ideas used here for choosing between different classes of correlations are primitive. Both experience and theory will be needed.

Our experience so far suggests strongly that a “second stage importance function” for pairs can be defined that is distinct from the original importance function. This new function would be used, for example, to bias the dynamics of pairs to prevent their annihilation. In general, its use should improve the efficiency and scalability to large systems of the method. At the moment, only very preliminary ideas exist about the nature of such a new pair importance function.

It would be useful to find a way to incorporate this basic idea into Green’s Function Monte Carlo so as to have a fermion algorithm with no time-step error. The new methodology should prove applicable to Monte Carlo methods for systems at finite temperature such as path integral methods.

Finally, we conjecture that the idea of variable correlation for pairs of systems will be applicable to other forms of Quantum Monte Carlo. The challenge posed by treating fermions can be viewed as the need to break an algorithmic symmetry between signed entities, and it may be possible to treat other calculations in this class in the same way.

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Tables

Table I

Eigenvalues obtained from the numerical relaxation program for the simple harmonic oscillator

Δx	cutoff	EIG
0.200000	5.90000	1.9977403871
0.100000	5.95000	1.9994382021
0.100000	6.55000	1.9994382022
0.099160	5.90000	1.9994476213

TABLE II

Eigenvalues obtained from the Monte Carlo program for the simple harmonic oscillator

pairs		steps		δ		EIG	
500	2000	2000	200000	0.100	0.040	0.040	2.011227 (482)
1000	2000	2000	400000	0.100	0.040	0.020	2.005030 (312)

TABLE III

Potential Centers for Problem A

0.00000	3.00000	0.00000	-3.00000	1.73202	1.00000
-1.73202	-1.00000	0.86603	-0.50000	-0.86603	0.50000

TABLE IV

Monte Carlo results for problem A

pairs				steps				δ	EIG
1000	4000	4000	80000	0.100	0.040	0.040	1.154122	(410)	
2000	4000	4000	80000	0.100	0.040	0.040	1.153422	(225)	
1000	4000	8000	160000	0.100	0.040	0.020	1.152503	(727)	
2000	4000	8000	80000	0.100	0.020	0.010	1.152575	(1052)	

TABLE V

Potential Centers for Problem B.

0.00000	0.90000	0.00000	-0.90000	0.51960	0.30000
-0.51960	-0.30000	0.25981	-0.15000	-0.25981	0.15000

TABLE VI

Monte Carlo results for problem B

pairs				steps				δ	EIG
500	2000	2000	200000	0.100	0.040	0.040	1.747695	(068)	
1000	2000	2000	500000	0.100	0.040	0.020	1.747398	(054)	

TABLE VII

Potential Centers for Problem C.

8.00000	0.00000	-8.00000	0.00000	7.74250	-1.46900
-7.74250	1.46900	7.21210	-2.86260	-7.21210	2.86260
6.42430	-4.12820	-6.42430	4.12820	5.40510	-5.21580
-5.40510	5.21580	4.19090	-6.07970	-4.19090	6.07970
2.82770	-6.68110	-2.82770	6.68110	1.37060	-6.99020
-1.37060	6.99020	-0.11850	-6.98820	0.11850	6.98820
-1.57270	-6.66970	1.57270	6.66970	-2.92280	-6.04350
2.92280	6.04350	-4.10060	-5.13450	4.10060	5.13450
-5.04210	-3.98330	5.04210	3.98330	-5.69200	-2.64620
5.69200	2.64620	-6.00740	-1.19410	6.00740	1.19410
-5.96190	0.29050	5.96190	-0.29050	-5.54960	1.71660
5.54960	-1.71660	-4.78780	2.98980	4.78780	-2.98980
-3.71960	4.01810	3.71960	-4.01810	-2.41450	4.71930
2.41450	-4.71930	-0.96680	5.02880	0.96680	-5.02880
0.50730	4.90830	-0.50730	-4.90830	1.87660	4.35370
-1.87660	-4.35370	3.00470	3.40270	-3.00470	-3.40270

TABLE VIII

Monte Carlo results for problem C

pairs		steps		δ			EIG
2000	20000	5000	50000	0.500	0.200	0.100	1.023668 (519)
1000	20000	5000	100000	0.500	0.200	0.200	1.030588 (431)

Caption for Figure 1. Centers, r_k , for the wavefunction specified in Equation (17) for the problem described in Table VII.