

## Diffusion Quantum Monte Carlo

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Citation: [Computers in Physics](#) **4**, 662 (1990); doi: 10.1063/1.4822960

View online: <https://doi.org/10.1063/1.4822960>

View Table of Contents: <https://aip.scitation.org/toc/cip/4/6>

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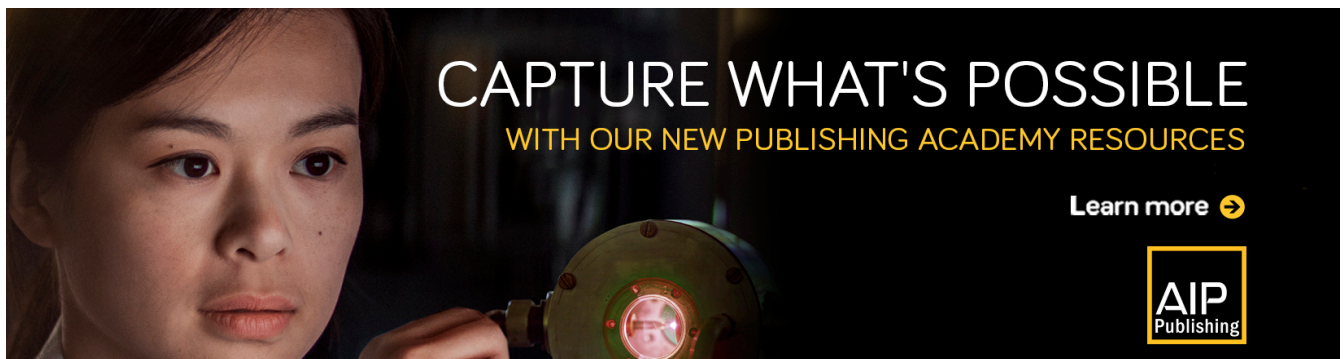
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# Diffusion Quantum Monte Carlo

Peter J. Reynolds, Jan Tobochnik, and Harvey Gould

**M**onte Carlo has become a widely employed tool for studying phenomena as diverse as the interactions of subatomic particles to the flow of highway traffic. Although the use of Monte Carlo methods—generally involving the use of random numbers in a calculation—became practical only with the availability of computers, the ideas behind Monte Carlo already existed in the statistics community since the early 1900s. As an example, statisticians performed “model sampling” of distributions using tables of random numbers. The derivation of the Student’s  $t$  distribution<sup>1</sup> was aided by this use of Monte Carlo. But it was almost 50 years later and totally independently that physicists and mathematicians began to realize that difficult and otherwise intractable problems could be recast in terms of stochastic processes.

A seminal symposium<sup>2</sup> was held in 1949 where a now forgotten distinction was made between earlier work and the new Monte Carlo method, defined to be the application of stochastic methods to problems arising from *nonprobabilistic* contexts. Many workers preferred a still more restrictive definition allowing only approaches that involved a “swindle” such as importance sampling, i.e., a mapping that made the connection to the original problem more obscure. Ironically, most of the problems that were discussed involved the reformulation of analytical equations back to their probabilistic roots, e.g., the diffusion of particles. The main exception was due to Metropolis and Ulam<sup>3</sup> who, following a suggestion by Fermi, used Monte Carlo methods to compute the ground-state energy of the Schrödinger equation. Fermi<sup>2</sup> noted the similarity of the time-dependent Schrödinger equation to a diffusion equation and proposed that a suitable random walk process could be found. Ulam formulated a random walk on a lattice, with “reproduction” possible at each lattice site. These developments were the beginning of quantum Monte Carlo.

Although work continued into the 1950s, no improvements were found over more traditional numerical methods for treating quantum mechanics, and subsequently the approach faded from the scene for several years. However, in the 1960s Kalos developed a much more sophisticated Monte Carlo approach to quantum mechanics, now called Green’s function Monte Carlo (GFMC).<sup>4,5</sup> Later, in the 1970s, Anderson independently discovered how to solve certain problems in quantum

chemistry by using random walks.<sup>6</sup> In this context, he was the first to treat fermion problems by Monte Carlo. These two very similar Monte Carlo approaches also have a clear interpretation in terms of Feynman path integrals,<sup>7</sup> providing another point of view of the quantum nature of these Monte Carlo methods. A discussion of explicit path integral quantum Monte Carlo methods was given in an earlier column.<sup>8</sup>

The path integral approach and the Green’s function method differ mostly in how the kinetic energy operator  $T$  is treated. In path integral Monte Carlo,  $T$  becomes part of the potential between imaginary replica particles, while in GFMC its contribution is used to cause diffusion (a random walk). Our goal in this column is to give an introductory exposition of the Green’s function Monte Carlo method.

Interest in GFMC as a computational tool arises from its ability to yield an in principle exact stochastic solution to the many-body Schrödinger equation, particularly in a continuum. Ground-state<sup>6,9</sup> and excited-state energies<sup>10</sup> as well as other properties<sup>11</sup> of quantum systems are readily obtained. Because the GFMC method often gives highly accurate answers, it thereby provides a check on other calculational procedures. Among its limitations, which it shares with path integral Monte Carlo, are the lack of a stable, exact algorithm for fermions; large CPU requirements (characteristic of Monte Carlo in general); and the difficulty of simulating atoms with large atomic number. The latter problem is related in part to critical slowing down, which has been discussed in a previous column in the context of spin systems.<sup>12</sup>

To make our discussion concrete, we begin by providing a simple presentation of GFMC in a form often called diffusion quantum Monte Carlo. If we rewrite the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi \quad (1)$$

in *imaginary* time, we will see that the two terms on the right-hand side can be interpreted as a diffusion term with a diffusion constant  $D = \hbar^2/2m$  and a rate term of the form  $-V\Psi$ . Diffusion, of course, is the continuum limit of a random walk. In the absence of diffusion, (1) is a rate equation describing a random decay or growth process. Both terms separately have analytical solutions and describe processes that have a random character. We will use this knowledge in the following. But how is the solution of the imaginary time equation related to the original Schrödinger equation? Have we done something drastic by considering imaginary time? We can under-

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stand what we have done by looking at the formal solution to (1):

$$\Psi(\mathbf{r}, t) = \sum_i \phi_i(\mathbf{r}) e^{-iE_i t/\hbar}, \quad (2)$$

where  $\mathbf{r}$  is a  $3N$ -dimensional vector representing the coordinates of the  $N$  particles, and  $\phi_n$  and  $E_n$  are the eigenfunctions and eigenvalues, respectively, of the time-independent Schrödinger equation. We see that for imaginary time, (2) becomes a sum of exponentially decaying terms. Thus instead of a time-dependent superposition of states, imaginary time acts as a projector that at large time projects out the lowest energy state.

Since a constant can be added to the potential without changing the form of the  $\phi_i$ , we can shift the zero of energy to  $E_0$  in order that the ground state survives. Putting these considerations together, we now rewrite (1) in imaginary time by substituting  $\tau = it/\hbar$  and shifting the energy:

$$\frac{\partial \Psi}{\partial \tau} = D \nabla^2 \Psi - (V - E_0) \Psi = -H \Psi, \quad (3)$$

with  $H = T + (V - E_0)$ . For simplicity we will absorb  $\hbar$  into the unit of time and write  $t$  instead of  $\tau$  in the following.

Equation (3) has a formal Green's function or operator solution of the form

$$G = e^{-iH}, \quad (4a)$$

with

$$\Psi(t) = G \Psi(0). \quad (4b)$$

$G$  can be interpreted as the probability of moving from  $\mathbf{r}$  to  $\mathbf{r}'$  in time  $t$  by writing it in the position representation:

$$G(\mathbf{r} \rightarrow \mathbf{r}', t) = \langle \mathbf{r}' | e^{-i(T + V - E_0)t} | \mathbf{r} \rangle. \quad (5)$$

One of Kalos' important contributions was to show how to use Monte Carlo to sample from the exact  $G$ , even when it is unknown.<sup>4,5</sup> This method may be described as a Monte Carlo iteration of a Fredholm integral equation, starting with the exact  $G_0$  for a simple potential  $V_0$ . Monte Carlo methods are used to sum the terms in an infinite series by a random walk. Rather than describing this fairly sophisticated procedure, we will discuss the often-used short-time approximation to  $G$ . In this approximation we can take advantage of the exact solutions to the diffusion and rate problems to write an explicit analytical form<sup>9,13</sup> for  $G$ . We can approximate  $G$  in (5) to  $O(t)$ , for example, with the error resulting from the fact that  $V$  and  $T$  are noncommuting operators. The resulting short-time approximation to  $G$  is

$$\begin{aligned} G(\mathbf{r} \rightarrow \mathbf{r}', \Delta t) &\cong \langle \mathbf{r}' | e^{-\Delta t V/2} e^{-\Delta t T} e^{-\Delta t V/2} | \mathbf{r} \rangle e^{+\Delta t E_0} \\ &= \exp\{ -(\Delta t/2)[V(\mathbf{r}') + V(\mathbf{r})] \\ &\quad + \Delta t E_0 \} \langle \mathbf{r}' | e^{-\Delta t T} | \mathbf{r} \rangle \\ &\equiv w(\mathbf{r}, \mathbf{r}'; \Delta t) G_D(\mathbf{r} \rightarrow \mathbf{r}', \Delta t), \end{aligned} \quad (6)$$

where  $w(\mathbf{r}, \mathbf{r}'; \Delta t)$  is the rate of decay or birth of random walkers and is given by

$$w(\mathbf{r}, \mathbf{r}'; \Delta t) = \exp\{ -(\Delta t/2)[V(\mathbf{r}') + V(\mathbf{r})] + \Delta t E_0 \}. \quad (7a)$$

The propagator  $G_D$  is simply the solution for ordinary diffusion:

$$G_D(\mathbf{r} \rightarrow \mathbf{r}', \Delta t) = (4\pi D \Delta t)^{-3N/2} e^{-(\mathbf{r}' - \mathbf{r})^2/4D \Delta t}. \quad (7b)$$

We use  $\Delta t$  in the argument of  $G$  to remind us that the form (6) is applicable only for small time intervals.

The procedure given in the following will simulate the imaginary time Schrödinger equation and yield an estimate of the ground-state energy and eigenfunction.

0. Begin with a set of  $M$  configurations of the coordinate vector  $\mathbf{r}$ . Each configuration is a set of  $3N$ -dimensional points representing the positions of all the quantum particles being considered and is essentially a "snapshot" of the coordinates. There is no lattice so the positions are continuous. It helps to choose these positions so that they are in regions of space where the wave function is expected to be reasonably large. The value of  $M$  will depend on the problem being treated and the precision desired, but values in the range from 100 to 1000 are reasonable. Each of these initial configurations has a local time  $t = 0$ .

1. Choose one of the  $M$  configurations and displace each of the coordinates from  $\mathbf{r}$  to  $\mathbf{r}'$ . The change is chosen from a Gaussian distribution with a width  $2D \Delta t$  and zero mean. This change corresponds to the diffusion step given by (7b). Choose the change in time,  $\Delta t$ , to be small so that the approximation given by (6) is accurate. Update the local time of the new configuration by  $\Delta t$ .

2. Weight the configuration  $\mathbf{r}'$  by  $w(\mathbf{r}, \mathbf{r}'; \Delta t)$  to complete the Green's function in (6). A convenient form of weighting that in many instances increases sampling efficiency is called branching. The idea is to represent the weight by what are initially duplicate random walkers. For example, if  $w \approx 2$ , we might produce two walkers at  $\mathbf{r}'$ , where there was previously only one. On the next update the two walkers will in general go to different places because of the random character of the moves. The trail of the random walk will look much like a branched polymer, although there is no self-avoiding constraint. In order to implement branching correctly, we must make an integer number of copies of the snapshot that is equal on average to the real number  $w$ . A simple way to implement branching is to take the integer part of  $(w + \xi)$ , where  $\xi$  is a uniform random number in the interval  $0 \leq \xi < 1$ . Note that the number of copies can be any nonnegative integer including zero which corresponds to a termination of the random walk. Each of the copies has the same local time. See Fig. 1 for a schematic representation of the possible Monte Carlo steps.

3. Repeat step 1 for all members of the ensemble, thereby generating a new ensemble at a later time  $\Delta t$  with a different number of snapshots or configurations. One iteration of the ensemble is equivalent to performing the integration

$$\Psi(\mathbf{r}', t) = \int d\mathbf{r} G(\mathbf{r} \rightarrow \mathbf{r}', \Delta t) \Psi(\mathbf{r}, t - \Delta t). \quad (8)$$

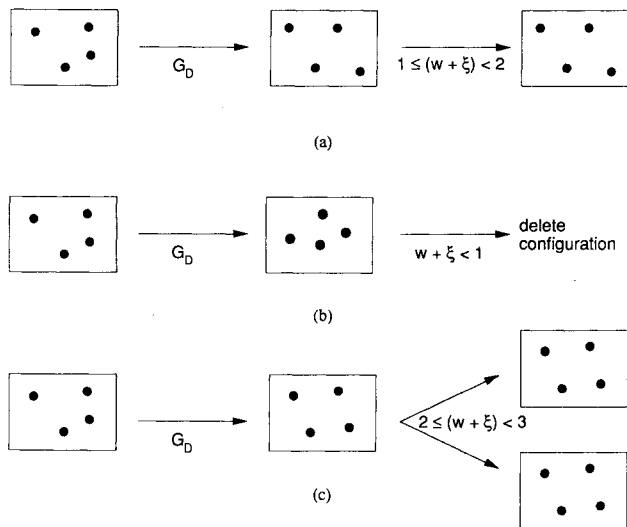


Fig. 1. Illustration of one Monte Carlo step. The particle coordinates are changed according to the short-time approximation, i.e., using the diffusion Green's function,  $G_D$ . The value of the function,  $w + \xi$ , where  $\xi$  is a random number on the interval  $0 \leq \xi < 1$ , determines whether (a) one configuration is kept; (b) the configuration is deleted; or (c) multiple copies of the configuration are made. In the case shown in (c), the new configuration plus one copy is made.

4. Independently of the original ensemble,  $\Psi(\mathbf{r}, t)$  is a solution to (3). However, as we discussed, it is necessary to iterate (8) to asymptotically large  $t$  to converge to the ground-state distribution. Thus steps 1–3 must be repeated for many thousands of Monte Carlo steps. Recall that we must adjust  $E_0$  to keep the ground-state population from decaying to zero. If  $E_0$  is too small, the population will grow instead. By adjusting  $E_0$  to keep the population asymptotically stable, we can estimate the ground-state energy. However, to keep the simulation stable,  $E_0$  is updated infrequently, usually no more than every 100 Monte Carlo steps in practical applications. To adjust  $E_0$ , we can replace it with  $E_0 - a[M(t) - M(0)]/[\Delta t M(0)]$ , where  $M(t)$  is the number of configurations at the current time,  $M(0)$  is the initial number of configurations that you wish to maintain, and  $a$  is a proportionality factor. If the number of configurations changes too quickly,  $a$  can be reduced. The snapshots generated once steady state is reached are samples of the ground-state wave function.

Unfortunately, the above procedure can be very inefficient, due in part to the branching process. When the potential becomes large and negative (recall that the Coulomb potential is singular whenever two particles approach one another), the number of copies of a random walker near this singularity would become exceedingly large. Thus to complete the next time step would require a vast number of walkers, and the simulation would bog down. In general, efficiency can be improved when known information is incorporated into a simulation. Kalos and coworkers found a simple, but remarkably effective importance sampling scheme,<sup>14</sup> that incorporates infor-

mation provided by a guess of the wave function, i.e., a trial wave function  $\Psi_T(\mathbf{r})$ . In this method the imaginary-time Schrödinger equation is expressed in terms of the product  $f = \Psi_T \Psi$ . The result for  $f$  is

$$\frac{\partial f}{\partial t} = D \nabla^2 f - D \nabla \cdot [f \mathbf{F}(\mathbf{r})] + [E_0 - E_L(\mathbf{r})]f, \quad (9)$$

where  $E_L = H\Psi_T/\Psi_T$  is the “local” energy, and  $\mathbf{F} = 2\nabla \ln \Psi_T$ . To verify (9) substitute  $f = \Psi_T \Psi$  and perform the vector derivatives. You will find that (9) reduces to the Schrödinger equation multiplied by  $\Psi_T$ . The structure of (9) is similar to (3). In particular it resembles a diffusion plus a branching process, but now there is a drift velocity imposed on the diffusion. The singularities in the branching factor are now almost gone, since  $E_L$  (unlike  $V$ ) is almost a constant. In fact,  $E_L$  approaches a constant as  $\Psi_T \rightarrow \Psi$ . Furthermore, the drift term now guides the walk preferentially into regions of space where the wave function is large.

We can write (9) for the Green's function as

$$\frac{d\tilde{G}}{dt} = -\tilde{H}\tilde{G} = -(\tilde{T} + \tilde{V})\tilde{G}, \quad (10)$$

with

$$\tilde{T} = -D\nabla^2 + D\nabla \cdot \mathbf{F} + D\mathbf{F} \cdot \nabla \quad (11a)$$

and

$$\tilde{V} = E_L - E_0. \quad (11b)$$

We can now follow steps similar to those taking us from (4) to (7) to obtain

$$\tilde{G}(\mathbf{r} \rightarrow \mathbf{r}', \Delta t) = \tilde{w}(\mathbf{r}, \mathbf{r}'; \Delta t) \tilde{G}_D(\mathbf{r} \rightarrow \mathbf{r}', \Delta t), \quad (12)$$

where the weight  $\tilde{w}$  is now given by

$$\tilde{w}(\mathbf{r}, \mathbf{r}'; \Delta t) = \exp\{- (\Delta t / 2) [E_L(\mathbf{r}) + E_L(\mathbf{r}')] + \Delta t E_0\} \quad (13)$$

and the propagator  $\tilde{G}_D$  is given by

$$\begin{aligned} \tilde{G}_D &= \langle \mathbf{r}' | \exp(-\Delta t \tilde{T}) | \mathbf{r} \rangle \\ &= (4\pi D \Delta t)^{-3N/2} \\ &\quad \times \exp\{[\mathbf{r}' - \mathbf{r} - D \Delta t \mathbf{F}(\mathbf{r})]^2 / 4D \Delta t\}. \end{aligned} \quad (14)$$

$\tilde{G}_D$  represents the propagator for diffusion with a drift and is the solution to (9) without the branching term. We see that the importance sampling procedure is essentially the same as the original method presented above, except that the diffusion now has a superimposed drift, and the branching is modified. The simulation procedure remains essentially the same, although  $E_L$  and  $\mathbf{F}$  need to be computed at each time step to evaluate  $\tilde{w}$  and  $\tilde{G}_D$ , respectively. The modified procedure can be summarized as follows:

0. Choose an initial ensemble of configurations by choosing the initial configurations according to the probability  $\Psi_T$ .<sup>2</sup> One way to obtain this ensemble is to use the Metropolis algorithm.<sup>15</sup> Start with an initial configuration,  $\mathbf{r}$ . Then randomly change each coordinate in  $\mathbf{r}$  to a new configuration  $\mathbf{r}'$ . If  $[\Psi_T(\mathbf{r}')]^2 > [\Psi_T(\mathbf{r})]^2$ , then accept the change, otherwise compute the ratio,  $P = [\Psi_T(\mathbf{r}')]^2 / [\Psi_T(\mathbf{r})]^2$ , and a random number,  $\xi$ , uniformly distributed between 0 and 1. If  $P > \xi$ , then accept the configuration, otherwise reject it. Repeat this procedure for a number of moves to reach equilibrium. Equilibrium is reached when the average energy has settled down. Now choose from among the equilibrium configurations a set of  $M$  initial configurations. For example, if we update the configurations  $10M$  times we can choose every 10th configuration for one of our initial configurations.

1. Choose a configuration and displace the  $3N$ -dimensional coordinate  $\mathbf{r}$  to  $\mathbf{r}'$  by choosing a random number from a Gaussian distribution with a width  $2D \Delta t$  and mean of zero. To impose the drift, add a displacement of  $D \Delta t \mathbf{F}(\mathbf{r})$ . The effect of the drift term is to push the random walk away from unimportant regions where  $\Psi_T$  is small.

2. Weight the new configuration  $\mathbf{r}'$  by  $\tilde{w}(\mathbf{r}, \mathbf{r}'; \Delta t)$  by making a number of copies of the snapshot equal to the integer part of  $(\tilde{w} + \xi)$ . If  $\Psi_T$  has been chosen close to the true  $\Psi$ ,  $E_L$  will be close to  $E_0$ , and the branching will be greatly suppressed.

3. Repeat step 1 for all the configurations. This step updates the product  $f$  in analogy to (8), namely,

$$f(\mathbf{r}', t) = \int d\mathbf{r} \tilde{G}(\mathbf{r} \rightarrow \mathbf{r}', \Delta t) f(\mathbf{r}, t - \Delta t). \quad (15)$$

4. Repeat steps 1–3 for enough iterations to first reach equilibrium, and then to sample from the steady-state distribution.

The above procedure will provide a good estimate for the ground-state energy and the product  $\Psi_T \Psi$ , where  $\Psi$  is the exact wave function. If the trial wave function is a good approximation to  $\Psi$ , then one also can obtain good estimates of other quantities as well, such as various moments of the charge distribution or potential energy surfaces for molecular interactions. However, the reliability of these other estimates is limited by the fact that we are sampling from  $\Psi_T \Psi$  rather than  $\Psi^2$ . There are, however, algorithms that sample from  $\Psi^2$  when necessary. The generalization of the Green's function procedure to obtain excited states is also possible but a bit more difficult.<sup>10</sup>

With or without importance sampling, a nagging problem arises when quantum statistics is considered. Specifically for fermions, e.g., electrons, the wave function must be antisymmetric. Therefore, when more than one electron is in the same spin state, the wave function must change sign somewhere. This requirement is troublesome if we wish to interpret (3) and (9) as diffusion equations,

because the density of diffusers, or walkers, must be positive. How to handle this requirement is not fully resolved, though several approaches have been developed.<sup>16</sup> A generally good approximation for treating (9) follows from noting that the distribution  $f$  will always remain positive if  $\Psi$  and  $\Psi_T$  change signs together. This behavior is readily accomplished by forcing the solution  $\Psi$  to vanish at the nodes of  $\Psi_T$ . This "fixed-node approximation"<sup>9,13,16</sup> is variational in nature, i.e., the energy thus derived will be an upper bound to the true energy. Several other methods have been devised to treat fermions, though all appear to contain some drawbacks. The fixed-node approach has the virtue of being simple, stable, variational, and generally accurate. The use of several trial functions, or optimizing parameters in a single  $\Psi_T$ , can indicate the order of magnitude of the approximation being made.

The method described in this column is one of many that have been designed to tackle quantum mechanical problems.<sup>17</sup> In a future column we hope to discuss the Green's function Monte Carlo method in which the Green's function is sampled directly rather than by a short-time approximation.

## Suggestions for Further Study

1. Carry out the "naive" diffusion quantum Monte Carlo method for the one-dimensional harmonic oscillator. If you have already considered the harmonic oscillator using the path integral method discussed in Ref. 8, compare the efficiency and ease of programming between the two methods. We have found accuracy at the 5%–10% level using  $\Delta t = 0.01$ ,  $M = 100$ , 1000 MC steps and an adjustment of the energy every 20 MC steps with the proportionality factor  $a = 0.1$ . Include a nonlinear perturbation to the harmonic oscillator potential and determine the change in the ground-state energy. Other one-dimensional problems can be tried for comparison. Gaussian random numbers can be obtained using the Box-Muller algorithm. Generate two uniform deviates  $0 \leq r_1, r_2 \leq 1$  and compute  $A = \sqrt{-4D \Delta t \ln r_1}$ ,  $\theta = 2\pi r_2$ ,  $g_1 = A \sin \theta$ , and  $g_2 = A \cos \theta$ . The quantities  $g_1$  and  $g_2$  are normalized Gaussian random variates, each with zero mean and variance of  $2D \Delta t$ . Remember that the number of configurations changes with time due to branching. Because we want to update all the configurations at the same local time before updating configurations with a later local time, we must keep track of the time for each configuration. One way is to have a variable  $M$  represent the number of configurations at a particular time. We then run through each of these  $M$  configurations changing their coordinates and sometimes duplicating them. The duplicates can be given labels greater than  $M$  so that we know not to update them until the next time step. If we delete a configuration, it is useful to replace it in the array with a configuration from the end of the list. After we have finished updating all  $M$  configurations, we can change  $M$  to the new total number of configurations and begin again.

2. Recompute the energy of the harmonic oscillator using the importance sampling method. Use the importance function  $\Psi_T = e^{-\beta x^2}$ , and choose various values of  $\beta$ . Plot the statistical error obtained versus  $\beta$ . How much variance reduction can you achieve relative to the naive algorithm? Note that for this choice of  $\Psi_T$  a value of  $\beta$  exists that yields the exact ground-state wavefunction. This occurrence is not possible in practical applications. Consider another form of the trial wavefunction that does not have a form identical to the exact ground state.

3. Write a program to implement the "naive" simulation procedure for the hydrogen atom. Repeat the procedure for helium. Estimate the ground-state energy in each case.

4. Recompute the energy of the hydrogen atom using the importance sampling method. Use the importance function  $\Psi_T = e^{-\beta r}$ , and choose various values of  $\beta$ . (Note that  $\beta = 1$  gives the exact wave function.) Plot the statistical error versus  $\beta$ . Is there a value for  $\beta$  that corresponds to the first problem, where no importance sampling was used? How much variance reduction can you achieve in comparison to the naive algorithm?

5. A more formal method of computing the energy than looking for the value of  $E_0$  that keeps the population stable is to sample the local energy over the random walk once equilibrium has been reached. Its expectation value will also be  $E_0$ . Can you demonstrate this property of  $E_L$ ?

Redo Problem 4 with this method of computing the ground-state energy.

Please send us your results and your comments for further columns. Programs relevant to the suggested problems are available from the authors in True BASIC for IBM PC compatibles and Macintosh computers as well as in FORTRAN. Please address comments and requests to hgould@clarku, tobochnik@hey1.kzoo.edu, or reynolds@ocnr-hq.navy.mil. Future columns are planned on cellular automata, quantum chaos, and classical spin models. ■

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