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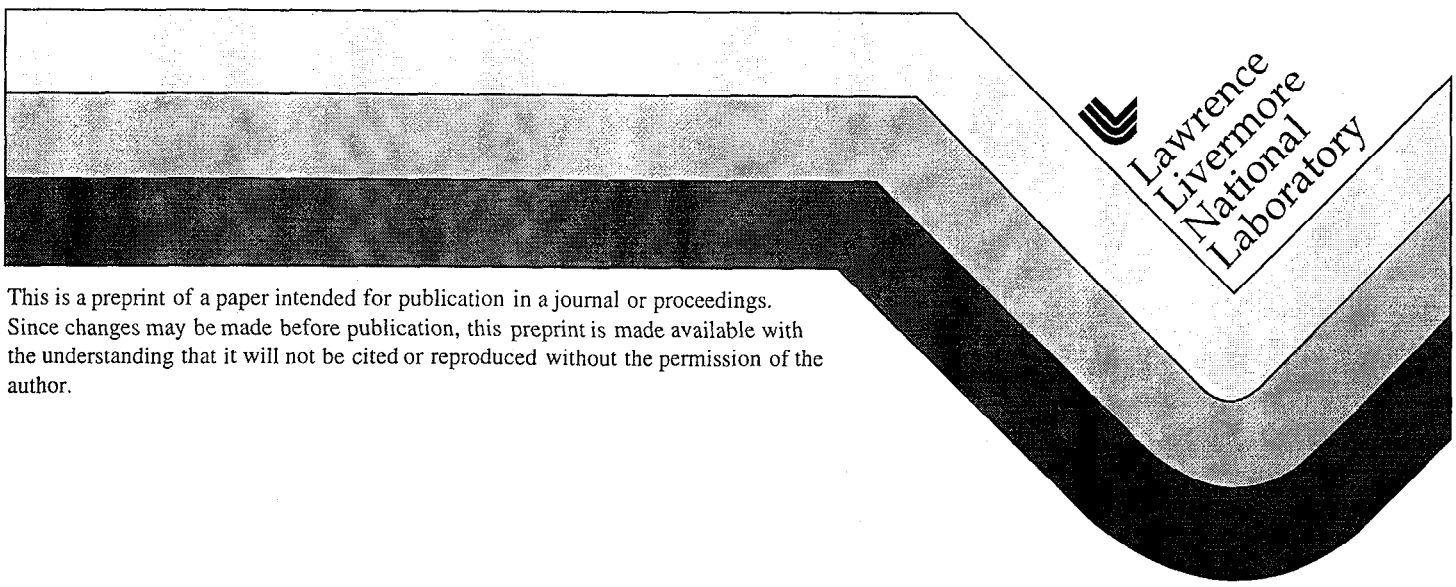

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Abstract

We review the fundamental challenge of fermion Monte Carlo for continuous systems, the "sign problem". We seek that eigenfunction of the many-body Schrödinger equation that is antisymmetric under interchange of the coordinates of pairs of particles. We describe methods that depend upon the use of correlated dynamics for pairs of correlated walkers that carry opposite signs. There is an algorithmic symmetry between such walkers that must be broken to create a method that is both exact and as effective as for symmetric functions. In our new method, it is broken by using different "guiding" functions for walkers of opposite signs, and a geometric correlation between steps of their walks. With a specific process of cancellation of the walkers, overlaps with antisymmetric test functions are preserved. Finally, we describe the progress in treating free-fermion systems and a fermion fluid with 14 ^{3}He atoms.

1 Introduction

Monte Carlo methods have provided the most powerful numerical tools for quantum many-body physics[1,2]. Since they deal effectively with many- dimensional quadrature, they permit a potentially fully-correlated wave function or density matrix to be used. In variational Monte Carlo, one introduces trial wave functions or density functions with explicitly chosen correlations built in. By minimizing some variational functional of these, one can obtain, for example, an optimal energy or free energy within the framework of the given class of trial functions, and also an indication whether or not the assumed correlations are realistic. Treating fermionic systems with explicitly antisymmetrized trial functions is usually not difficult.

By contrast, the methods that can, in principle, solve quantum problems exactly, namely Green's function Monte Carlo (GFMC), Diffusion Monte Carlo (DMC), or Path Integral Monte Carlo (PIMC) depend upon guessed properties of the many-body correlation only in their computational efficiency, if at all. They are capable of giving, at least for moderate size bosonic systems, answers with no uncontrolled approximations. Unfortunately, most interesting systems– electronic, ^{3}He, and nuclear– are made up of fermions, and the exact treatment of such systems has been impeded for years by the notorious "sign problem."

This paper is concerned with the nature of this challenge to computational mathematics and physics, and with a new proposal for solving it with which we have recently been experimenting. Broadly speaking, the difficulty can be characterized in different ways, but the outcome is the exponential decay of signal to noise, a kind of statistical instability. Thus, whereas a bosonic calculation has a statistical error that decreases asymptotically with computation time, t, as $1/\sqrt{t}$, a fermionic calculation naively pursued in the same way will exhibit an error that falls as $1/\log(t)$.

One straightforward way of understanding the nature of the difficulty is to recall that in GFMC or DMC, the random walks serve to filter out the higher energy modes of some trial or initial distribution, so that for very large imaginary time, the probability distribution of the random walkers is given by the ground state, which for potentials invariant under particle exchange is also the symmetric (bosonic) ground state.

The essence of GFMC or DMC can be expressed in the following way: One constructs a random walk that generates wave functions biased with a "trial" or "guiding" function $\psi_G(\vec{R})$. Assuming a basis $\phi_k(\vec{R})$, of eigenfunctions of the Hamiltonian $\hat{H}$, having eigenvalues E_k, then as a function of imaginary time τ, the walk generates a density of walkers according to

$$f(\vec{R},\tau) = \psi_G(\vec{R}) \sum_k a_k \exp[(E_T - E_k)\tau]\phi_k(\vec{R}) \tag{1}$$

where E_T is some trial eigenvalue. Asymptotically, $f(\vec{R},\tau)$ is dominated by the eigenfunction ϕ_0 with smallest eigenvalue E_0.

In a Monte Carlo calculation of this kind, we "project" quantities of interest by calculating weighted integrals with some trial function, say $\psi_T(\vec{R})$. For example, to calculate the energy eigenvalue, E_0, we write the Schrödinger equation:

$$\hat{H}\psi_0(\vec{R}) = E_0\psi_0(\vec{R}) \tag{2}$$

Now multiply both sides by $\psi_T(\vec{R})$, integrate over all $\vec{R}$, and solve for E_0 using

the property that $\hat{H}$ is hermitian. The result is

$$E_0 = \frac{\int \psi_0(\vec{R})\hat{H}\psi_T(\vec{R})d\vec{R}}{\int \psi_0(\vec{R})\psi_T(\vec{R})d\vec{R}} \tag{3}$$

For large τ, we may replace this by

$$E_0 = \frac{\int \frac{f(\vec{R},\tau)}{\psi_G(\vec{R})}\hat{H}\psi_T(\vec{R})d\vec{R}}{\int \frac{f(\vec{R},\tau)}{\psi_G(\vec{R})}\psi_T(\vec{R})d\vec{R}} \tag{4}$$

and finally, following the theory of Monte Carlo and given that the density of walkers is $f(\vec{R},\tau)$, replace the integrals by a sum over all positions $\vec{R}_m$ of walkers at large τ:

$$E_0 = \frac{\sum_m \frac{\hat{H}\psi_T(\vec{R}_m)}{\psi_G(\vec{R}_m)}}{\sum_m \frac{\psi_T(\vec{R}_m)}{\psi_G(\vec{R}_m)}} \tag{5}$$

This is very effective for determining E_0 of bosonic systems. Formally, we may simply use an antisymmetric function $\psi_T(\vec{R})$, relying on the fact that the corresponding exact eigenfunction is present in the expansion of f. But the variance of these integrals contains the squares of $\hat{H}\psi_T(\vec{R})$ and $\psi_T(\vec{R})$, which are symmetric. Thus the signal to noise ratio of these integrals decays exponentially with time. The usual Monte Carlo strategy of continuing the random walk to improve statistics does not work effectively. It could be made to work if the growth of the symmetric ground state (and other low-lying states) relative to the fermionic state could be controlled. That was the motivation for introducing cancellation methods by Arnow et al. [3], but these scale badly because, in a small population of walkers, close encounters are rare in many dimensions.

The well known "fixed–node"[4,5] method, in which the random walk is terminated on the nodes of an antisymmetric trial function $\psi_T(\vec{R})$ provides a simple approximate scheme for limiting that growth. It is often a very good approximation.

Historically, it seemed surprising that fermionic Monte Carlo would prove so difficult, and there have been many attempts to solve it in diverse ways. Perhaps a clear understanding of the challenge has never been articulated. For that reason, we offer a brief discussion of these issues, phrased as a set of answers to the sense that "there ought to be an easy way out!"

One line of thinking has been that fermionic Monte Carlo is exact and easy in one spatial dimension: Why should it be hard in many? A straightforward answer is that the nodal surfaces are known exactly in one dimension, and can be used with the fixed-node method, now no longer an approximation. A complementary and more instructive answer is the following. Cancellation methods, mentioned above, will work very well if the walkers meet. They are guaranteed to do just that in one dimension, but walks in higher dimensions are guaranteed never to meet. We shall return later with a new approach that makes cancellation possible for many–body systems.

In a similar spirit, it has seemed plausible that if the fixed-node approximation is easy and often rather accurate, a small improvement ought to be straightforward. This has not been done yet. A plausible reason is that the Pauli principle– which demands that the wave function be antisymmetric– provides a global constraint on the solution, but the random walks that underlie GFMC or DMC are always local, depending only on functions of the immediate position $\vec{R}$ to determine the next moves. Clearly some sort of non-local knowledge must be used. Even an approximate nodal surface provides global information about the solution. Later, we propose the use of correlated walkers to create a degree of non-locality.

Finally, by way of concluding this analysis of the sign problem, we introduce a point of view that we have found very helpful in understanding what needs to be done, and in determining whether a proposed method will work, namely the "plus-minus symmetry". We introduce explicitly a set of walkers, $\{\vec{R}_m^+, \vec{R}_m^-\}$, that respectively add or subtract their contributions to statistical expectations, such as in Eq. (5). With the use of such signed walkers, that equation becomes

$$E_0 = \frac{\sum_m [\frac{\hat{H}\psi_T(\vec{R}_m^+)}{\psi_G(\vec{R}_m^+)} - \frac{\hat{H}\psi_T(\vec{R}_m^-)}{\psi_G(\vec{R}_m^-)}]}{\sum_m [\frac{\psi_T(\vec{R}_m^+)}{\psi_G(\vec{R}_m^+)} - \frac{\psi_T(\vec{R}_m^-)}{\psi_G(\vec{R}_m^-)}]} \tag{6}$$

Now define a new set of walkers by assigning

$$\vec{S}_m^+ = \vec{R}_m^-, \quad \vec{S}_m^- = \vec{R}_m^+, \tag{7}$$

i.e. simply exchanging the $+, -$ labels. If the dynamics is unchanged by this transformation, then asymptotically there will be as many populations near $\{\vec{S}_m^+, \vec{S}_m^-\}$ as there are near $\{\vec{R}_m^+, \vec{R}_m^-\}$, and the expectations of the sums in Eq. (7) will vanish, guaranteeing the unfavorable consequences of the sign problem. An effective method must break this plus-minus symmetry.

2 Correlated Pairs

Is is clear that independent walkers cannot break the plus-minus symmetry, so that some correlation among walkers is essential. That raises two questions: How large a group of walkers must be correlated? Is it possible to guarantee correct results in spite of the correlation?

In this paper, we consider only correlated pairs, and will demonstrate stable results with that limitation. As for the question of correct results, consider dynamics of a pair in which the behavior of both walkers is the same as that of a single free walker, except when they cancel. The integrals that occur in Eq. (6) are linear in the walker density and their expectations are therefore unchanged by correlation between walkers. A procedure to insure that the expectations will be unaffected by cancellation will be demonstrated below. If it is used, then any stable results are also correct [6].

The dynamics for which the behavior of one member is still correct are easily obtained within the context of DMC. Recall that the "diffusion step" consists of displacing a walkers by a $3N$-dimensional vector of Gaussians whose components have the same distribution everywhere. If we choose this vector for a negative walker to be correlated with that of a positive walker, we can preserve the correct "marginal dynamics" for both. A specific prescription is given below.

3 The Stochastic Dynamics

We apply the general ideas of "mirror potentials"[7], to the positive and negative walkers of a pair and introduce the following guiding functions[8].

Let $\psi_S(\vec{R})$ be some approximation to the symmetric ground state wave function of the system. Let $\psi_A(\vec{R})$ be a trial function for the lowest antisymmetric state. The guiding functions are:

$$\psi_G^{\pm}(\vec{R}) = \sqrt{\psi_S^2(\vec{R}) + c^2\psi_A^2(\vec{R})} \pm c\psi_A(\vec{R}) \tag{8}$$

These functions have the following important properties. a) they are both positive everywhere; (b) for small values of the parameter c, they are dominated by ψ_S, so that the branching of the two walkers are not very different; (c) each is a sum of a symmetric and an antisymmetric term, and the latter changes sign with c; (d) an odd permutation $\mathcal{P}$ transforms ψ_G as follows:

$$\psi_G^{+}(\mathcal{P}\vec{R}) = \psi_G^{-}(\vec{R}). \tag{9}$$

To analyze the consequences of cancellation, we start by projecting the average future contribution of a walker undergoing diffusion Monte Carlo in which it is advanced by $\delta\tau$ using a guiding function $\psi_G(r)$. After a total imaginary time τ, an eigenfunction $\phi_k(\vec{R}_0)$ evolves according to

$$\psi_G(\vec{R}_0)\phi_k(\vec{R}_0) \rightarrow e^{(E_T-E_k)\tau}\psi_G(\vec{R})\phi_k(\vec{R}). \tag{10}$$

To estimate $A(\vec{R}_0)$, the total expected future contribution of a walker currently at $\vec{R}_0$ to an estimator $a(\vec{R})/\psi_G(\vec{R})$, use the expansion of $\delta(\vec{R}-\vec{R}_0)$:

$$\begin{aligned}\delta(\vec{R}-\vec{R}_0) &= \sum_k \phi_k(\vec{R})\phi_k(\vec{R}_0) \\ &\rightarrow \sum_k e^{(E_T-E_k)\tau}\psi_G(R)\phi_k(\vec{R})\phi_k(\vec{R}_0)/\psi_G(\vec{R}_0)\end{aligned} \tag{11}$$

Then $A(\vec{R}_0)$ is obtained from Eq. (11) by multiplying by $a(\vec{R})/\psi_G(\vec{R})$ and integrating over all $\vec{R}$ and over τ from 0 to ∞. The result is

$$A(\vec{R}_0) = \frac{1}{\psi_G(\vec{R}_0)}\sum_k [\int a(\vec{R})\phi_k(\vec{R})d\vec{R}]\frac{\phi_k(\vec{R}_0)}{E_k-E_T} = \frac{A_1(\vec{R}_0)}{\psi_G(\vec{R}_0)}. \tag{12}$$

Diffusion of the walkers are correlated in the following way:

$$\vec{R}_n^+ = \vec{R}^+ + \vec{U}^+ \quad \vec{R}_n^- = \vec{R}^- + \vec{U}^-. \tag{13}$$

$\vec{U}^+$ contains $3N$ Gaussian random variables each of mean zero and variance $\delta\tau$. $\vec{U}^-$ is obtained by reflecting $\vec{U}^+$ in the perpendicular bisector of the vector $\vec{R}^+ - \vec{R}^-$. Then the overlapping distributions of next positions, $\vec{R}$, are added algebraically so as to allow positive and negative walkers to cancel.

$$G(\vec{R}'-\vec{R}) = \frac{\exp[-(\vec{R}'-\vec{R})^2/(2\delta\tau)]}{(2\pi\delta\tau)^{3N/2}} \tag{14}$$

is the probability density that describes diffusion.

Let

$$B^+(\vec{R}|\vec{R}^+), \quad B^-(\vec{R}|\vec{R}^-) \tag{15}$$

denote the branching factors that are applied to a positive and a negative walker respectively on arriving at $\vec{R}$.

Using Eq. (12) and Eq. (14) to calculate the expected future contributions of positive and negative walkers arriving at $\vec{R}$, we conclude that a positive walker

at $\vec{R}_n^+$ will survive and be used as a positive walker in the next time step with probability

$$P^+(\vec{R}_n^+;\vec{R}^+,\vec{R}^-) = \max\left[0, 1 - \frac{B^-(\vec{R}_n^+|\vec{R}^-)G(\vec{R}_n^+ - \vec{R}^-)\psi_G^+(\vec{R}_n^+)}{B^+(\vec{R}_n^+|\vec{R}^+)G(\vec{R}_n^+ - \vec{R}^+)\psi_G^-(\vec{R}_n^+)}\right] \quad (16)$$

In standard diffusion Monte Carlo, the branching factors, $B^+(\vec{R}|\vec{R}^+)$ and $B^-(\vec{R}|\vec{R}^-)$ depend only on the arrival point, $\vec{R}$, and are respectively

$$B^\pm(\vec{R}) = \exp\left\{\delta\tau\left[E_T - \frac{H\psi_G^\pm(\vec{R})}{\psi_G^\pm(\vec{R})}\right]\right\} \quad (17)$$

Branching is carried out for both walkers of a pair. An unpaired walker may appear; a simple method of recreating a pair is with probability one half generate a partner of opposite sign by interchanging the coordinates of two like-spin particles. Half the time the walker is discarded. That this is unbiased is justified with the following argument. The functions $a(\vec{R})$ that interest us here are antisymmetric. Hence the coefficients of ϕ_k in Eq. (12) vanish except for antisymmetric functions. That is,

$$A_1(\mathcal{P}\vec{R}) = -A_1(\vec{R}) \quad (18)$$

According to Eq. (9), $\psi_G^+(\mathcal{P}\vec{R}) = \psi_G^-(\vec{R})$, so that

$$A(\mathcal{P}\vec{R}) = -A(\vec{R}) \quad (19)$$

Therefore, the expected future score from a walker at $\mathcal{P}\vec{R}$ is the negative of that at $\vec{R}$. In our estimates, however, all future contributions will be subtracted, so that the net score is doubled by adding the new partner at $\mathcal{P}\vec{R}$. The factor of two is corrected by creating the pair with probability one half as indicated. Along with the fact that random walks are (marginally) correct, this treatment of cancellation and repairing guarantees that the expectation of future contributions to the numerator and denominator of Eq. (3) are unchanged.

The most important result in these calculations is the energy. We use the estimator of Eq. (6). The denominator $\mathcal{D}$ in that quotient is our best indicator of stability. If the plus-minus symmetry is not broken, one expects $\mathcal{D}$ to decay to zero in an imaginary time of order $\tau_c = 1/(E_A - E_S)$ where E_A and E_S are the antisymmetric symmetric energies respectively. By contrast a stable method will show $\mathcal{D}$ growing linearly with imaginary time.

We experimented first with free fermions, a stringent test of our method. We assume $\hbar = m = 1$, and a density $\rho = 0.5$ The exact fermionic ground state

N	E	$\sigma(E)$	T (m)	$\sigma^2(E) * T/N^3$	E_{ex}
7	2.900	0.004	7822	0.00036	2.912712
19	2.792	0.020	24346	0.00142	2.757454
27	3.131	0.050	25488	0.00323	2.763316

Table 1
Energies, errors and time scaling for a periodic system of N free fermions. T is the total CPU time (in minutes) of the runs performed. The exact analytic result E_{ex} is reported for comparison.

is a determinant of plane waves; the lowest symmetric state is constant. We chose the guiding function to be:

$$\psi_G^{\pm}(\vec{R}) = \sqrt{1 + c^2\varphi_A^2(\vec{R})} \pm c\varphi_A(\vec{R}) \tag{20}$$

where φ_A is a Slater determinant of one body functions $\chi_{\vec{r}_i}^{\vec{k}}$ of the following form:

$$\chi_{\vec{r}_i}^{\vec{k}} = \exp\left[i\vec{k} \cdot \left(\vec{r}_i + \lambda_B \sum_{j \neq i} \eta(r_{ij})\vec{r}_{ij}\right)\right] \tag{21}$$

The nodal structure of this departs from the exact depending on the parameter λ_B. In table I we report the results obtained from variational calculations and DMC-fixed-node for periodic systems of 7, 19, and 27 particles respectively.

In Table I we show the results for a system of N free fermions, with $N = 7, 14, 27$. We report the energy per particle computed with the algorithm described above, the estimated errors, and an estimate of the MC computational complexity. As can be seen, in the $N = 7$ case the result is lower than the exact value, while in the $N = 19$ and $N = 27$ the energy is biased toward higher values. We remark that these calculations have been performed with a strictly fixed population of 50 walkers. Indications from numerical experiments with a larger number of walkers are that the bias is strongly reduced. We will perform a systematic study of the dependence of the energy on the number of walkers. The computational complexity appear to grow faster than the N^3 which is expected from the computation of the Slater determinants alone. Within the present uncertainties our estimates are compatible with a power law with an exponent ~ 4.5. A sharper analysis of the scaling is also under way. We have also applied this algorithm to a system of 14 ^{3}He atoms in a periodic box at equilibrium density. With interatomic potentials, the wave function must include a Jastrow factor:

$$\psi_G^{\pm}(\vec{R}) = \varphi_S(\vec{R}) \left[\sqrt{1 + c^2\varphi_A^2(\vec{R})} \pm c\varphi_A(\vec{R})\right] \tag{22}$$

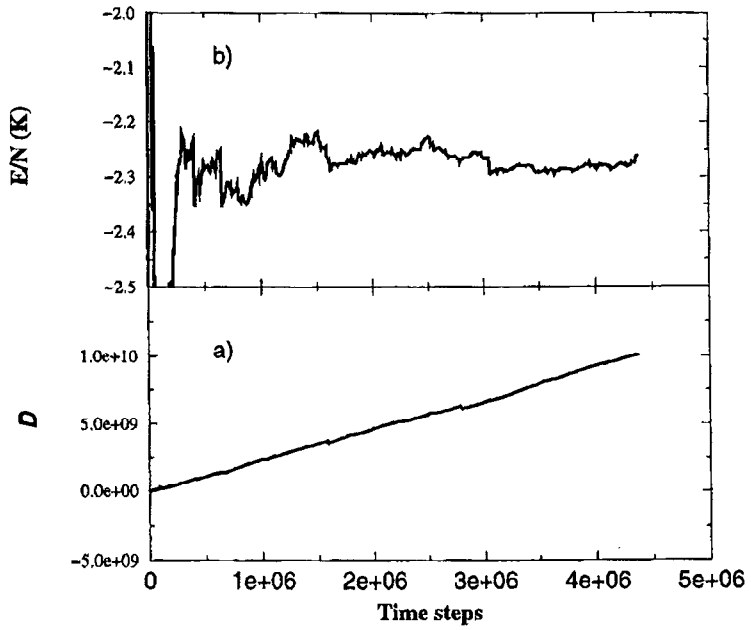

Fig. 1. a) Cumulative value of the denominator $\mathcal{D}$ and b) cumulative value of the energy per particle in a system of 14 ^{3}He atoms with periodic boundary conditions at equilibrium density.

The function φ_A is the same as for free fermions, while φ_S has the form $\varphi_S(\vec{R}) = \prod_{i<j} \exp[-(b/r_{ij})^5]$. Now the units of length are Å, while the energies are expressed in Kelvins. The density at which we performed our calculations is $\rho = 0.0216\text{Å}^{-3}$. The value of c is 0.02. In Fig. 1a we plot the cumulative value of $\mathcal{D}$. As can be seen, we have a very stable result. Fig. 1b shows the cumulative eigenvalue; the final average is $E_0 = -2.25 \pm 0.03K$. Neither extrapolation in imaginary time nor a check of the dependence on the number of walkers has been done yet. Thus the eigenvalue, though reasonable, is not yet definitive. We believe that neither the presence of realistic interatomic potentials nor many-body correlations alter the fundamental stability of the method.

4 Conclusions

We have proposed an approach to the Monte Carlo treatment of many-fermion systems in which different guiding functions for positive and negative walkers are used. A geometric correlation of the diffusive steps of the walks combines with the effect of the importance sampling to give random walks that exhibit statistical stability to very long imaginary times. This geometrical correlation is able to guide walkers together even in the configuration space of many

particles, a necessary property of an effective algorithm. The method has been successful with systems of as may as 27 fully polarized free fermions as well as a system of 14 atoms of ^{3}He with realistic potentials. In principle the correct dynamics for each walker plus correct form of the probability of cancellation of opposite walkers guarantees unbiased results. These experimental results suffer from known biases: The first versions of our programs do not carry out the exact sampling required. It seems clear, however, that an important step forward has been taken toward our goal of an exact method for many-fermion calculations.

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