Sign problem in the numerical simulation of many-electron systems

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We discuss the problems that arise in the numerical simulation of many-electron systems when the measure of the functional integrals is not positive definite. We present theoretical arguments and numerical data which indicate that the expectation value of the sign of the measure decreases exponentially as the inverse temperature β increases, unless the measure is forced to be positive by an explicit symmetry. We therefore conclude that a recent proposal for dealing with the sign problem due to Sorella *et al.* leads to an uncontrolled approximation. In the cases we have studied it is a good approximation for the ground-state energy, and we present a method for calculating the correction needed to make it exact. However, for some physical quantities, such as the d-wave pair field susceptibility, the neglect of signs can yield misleading results.

I. INTRODUCTION

Numerical simulations can be a powerful tool for the study of systems of strongly correlated electrons. However, in many problems of physical interest the functional integrals that are to be evaluated numerically do not have a positive definite measure. In this paper we discuss the problems that arise in simulations when the measure is not positive definite, and present data from simulations of the two-dimensional Hubbard model. We also discuss a recent suggestion for dealing with this sign problem due to Sorella *et al.*[1]

Numerical simulations have been performed at finite temperature within the grand canonical ensemble[2–4] and at zero temperature for a fixed number of electrons.[5,1,4] To carry out these simulations one must first integrate out the electron degree of freedom. This is possible if the Hamiltonian is quadratic in the electron creation and annihilation operators, or can be made so through a Hubbard-Stratonovich transformation. One is then left with an expression for the expectation value of a physical observable O of the general form

$$\langle O \rangle = \frac{\sum_x \rho(x) O(x)}{\sum_{x'} \rho(x')} . \tag{1}$$

Here $\sum_x$ represents either a set of integrals over continuous variables or a sum over discrete spin variables. For the grand canonical ensemble, the measure $\rho(x)$ is proportional to the well-known fermion determinants for the spin-up and spin-down electrons.[2]

If $\rho(x)$ is positive semidefinite, then the right-hand side of Eq. (1) can be evaluated by importance-sampling techniques. One generates a sequence of configurations $\{x\}$ with a probability distribution

$$P(x) = \frac{\rho(x)}{\sum_{x'} \rho(x')} , \tag{2}$$

and measures $O(x)$ in these configurations. There are a limited number of models for which one can prove that $\rho(x)$ is positive semidefinite. The single-band Hubbard model with a repulsive Coulomb interaction and a half-filled band is one example.[3] The Hubbard model with an attractive Coulomb interaction and electron-phonon models in which the phonon field couples identically to the spin-up and spin-down electrons are examples of models for which $\rho(x)$ is positive semidefinite for arbitrary fillings. In all cases that we are aware of, the positivity of $\rho(x)$ follows from a discrete symmetry of the model.

There are many models for which $\rho(x)$ is not positive semidefinite: the repulsive Hubbard model away from half-filling,[3] the attractive Hubbard model, and electron-phonon models in external magnetic fields are examples. For such models simulations can, in some cases, still be carried out. One can write

$$\rho(x) = |\rho(x)| S(x) , \tag{3}$$

with $S(x) = \pm 1$. Then, introducing the probability function

$$\tilde{P}(x) = \frac{|\rho(x)|}{\sum'_x |\rho(x')|} , \tag{4}$$

Eq. (1) can be rewritten as

$$\langle O \rangle = \frac{\langle OS \rangle_{\tilde{P}}}{\langle S \rangle_{\tilde{P}}} , \tag{5}$$

where $\langle\ \rangle_{\tilde{P}}$ indicates an average with respect to the probability distribution $\tilde{P}$. Equation (5) is a useful starting point for numerical simulations only if $\langle S\rangle_{\tilde{P}}$ is not "too small." Otherwise, there will be large cancellations in $\langle OS\rangle_{\tilde{P}}$ and $\langle S\rangle_{\tilde{P}}$, and statistical fluctuations will make an accurate evaluation of $\langle O\rangle$ extremely difficult.

As will be discussed in Sec. II, we expect that in calculations with the grand canonical ensemble $\langle S\rangle_{\tilde{P}}$ will go to zero exponentially as the inverse temperature β increases. In calculations of ground-state properties one uses the operator $\exp(-\frac{1}{2}\beta H)$ to project the ground-state wave function from a trial wave function. Again in the limit of large β, which is necessary for the projection, we expect $\langle S\rangle_{\tilde{P}}$ to go to zero exponentially. In Sec. III we present numerical results for the two-dimensional Hubbard model that are in accord with these expectations. We find that the rate at which $\langle S\rangle_{\tilde{P}}$ approaches zero depends strongly on the band filling and on the coupling.

Sorella *et al.*[1] have recently suggested that in calculations of ground-state properties there may be some fillings and parameter regimes for which the trial function can be chosen so that $\langle S\rangle_{\tilde{P}}$ will approach a constant as $\beta\rightarrow\infty$. In such cases they argue that some quantities of physical interest can be calculated by neglecting the sign of $\rho(x)$. They also present alternative, positive definite weight functions, which they argue will produce the same physical results for these quantities. We have repeated some of their calculations for the two-dimensional Hubbard model, and find that in all cases $\langle S\rangle_{\tilde{P}}$ approaches zero exponentially with increasing β. We are therefore led to the conclusion that their computational method is an uncontrolled approximation. However, in tests that we have made on small lattices for which we can compare Monte Carlo results with those obtained by exact diagonalization of the Hamiltonian, it does give a good approximation to the ground-state energy and some other physical quantities. Furthermore, one can calculate the difference in the ground-state energy obtained with and without signs very accurately by measuring the rate of exponential decay of the sign. There are corresponding calculations that allow one to determine the difference in any physical quantity calculated with and without signs, but they require high-precision measurements. Finally we show that the d-wave pairing susceptibility has very different behavior at low temperatures when calculated with and without inclusion of the signs. This example clearly illustrates the uncontrolled nature of the approximation.

II. THEORETICAL CONSIDERATIONS

We shall consider both calculations within the grand canonical ensemble and calculations of ground-state properties for a fixed number of electrons. In the former case the expectation value of a physical observable Q is given by

$$\langle O\rangle=\frac{\mathrm{tr}O\ e^{-\beta(H-\mu N)}}{\mathrm{tr}e^{-\beta(H-\mu N)}}\ , \tag{6}$$

where H is the Hamiltonian, μ the chemical potential, and β the inverse temperature. To obtain ground-state properties one replaces the traces in Eq. (6) by expectation values in a trial wave function with n electrons, $|\Psi_T^n\rangle$. Denoting the eigenvectors and eigenvalues of H in the n-electron sector by $|\psi_l\rangle$ and E_l, respectively, one can write

$$|\Psi(\beta/2)\rangle=e^{-1/2\beta H}|\Psi_T^n\rangle=\sum_l e^{-1/2\beta E_l}|\psi_l\rangle\langle\psi_l|\Psi_T^n\rangle\ . \tag{7}$$

Clearly, for large β, $|\Psi(\beta/2)\rangle$ becomes proportional to $|\psi_0\rangle$, and

$$\langle\psi_0|O|\psi_0\rangle=\lim_{\beta\rightarrow\infty}\frac{\langle\Psi(\beta/2)|O|\Psi(\beta/2)\rangle}{\langle\Psi(\beta/2)|\Psi(\beta/2)\rangle}\ . \tag{8}$$

The quantity

$$\langle\Psi(\beta/2)|\Psi(\beta/2)\rangle=\langle\Psi_T^n|\exp(-\beta H)|\Psi_T^n\rangle$$

plays the same role in simulations of ground-state properties as the partition function $\mathrm{tr}\exp[-\beta(H-\mu N)]$ does in the grand-canonical-ensemble simulations. The integrands of the path integrals for these quantities provide the probability distributions for the numerical simulations. We shall use the symbol Z for both of them.

In order to carry out numerical calculations it is necessary to integrate out the electron degrees of freedom. To this end one divides the region 0 to β into L imaginary-time slices of width $\Delta\tau$. If the Hamiltonian is not quadratic in the electron creation and annihilation operators, one makes it so by introducing a Hubbard-Stratonovich transformation on each time slice. The density operator $\exp(-\beta H)$ can then be written in the form

$$e^{-\beta H}=\sum_x e^{-\Delta\tau\mathcal{H}(L)}\cdots e^{-\Delta\tau\mathcal{H}(2)}e^{-\Delta\tau\mathcal{H}(1)}\ . \tag{9}$$

The effective Hamiltonian for the lth time slice, $\mathcal{H}(l)$, has the general form

$$\mathcal{H}(i)=\sum_{\sigma=\pm}c_{i,\sigma}^{\dagger}h_{i,j}^{\sigma}(x_l)c_{j,\sigma}\ , \tag{10}$$

where $c_{i,\sigma}^{\dagger}$ and $c_{i,\sigma}$ are the creation and annihilation operators for electrons on the ith lattice site with z component of spin σ, and x_l are the Hubbard-Stratonovich variables for the lth time slice. The Hubbard-Stratonovich field x_l will have one or more components on each lattice site. In electron-phonon models in which the fermions are coupled to the phonons by an interaction which is quadratic in the creation and annihilation operators, the Hubbard-Stratonovich field is replaced by a dynamical phonon field. In what follows we shall not distinguish between these fields, and refer to them both as Hubbard-Stratonovich fields.

Although the operator $\exp(-\beta H)$ is positive definite, the individual terms on the right-hand side of Eq. (9) in general are not. This is why the weight function $\rho(x)$ defined in Eq. (1) need not be positive definite although Z is. The traces over the electron degrees of freedom can be done explicitly for the grand canonical ensemble, and one finds that $\rho(x)$ can be written in the form[2]

$$\rho(x)=f(x)\det[I+e^{\beta\mu}A^{+}(x)]\det[I+e^{\beta\mu}A^{-}(x)]\ , \quad (11)$$

where $f(x)$ is positive definite and

$$A^{\sigma}(x)=e^{-\Delta\tau h^{\sigma}(x_L)}\cdots e^{-\Delta\tau h^{\sigma}(x_2)}e^{-\Delta\tau h^{\sigma}(x_1)}\ . \quad (12)$$

For the zero-temperature, fixed particle number, ground-state calculations,

$$\rho(x)=f(x)\det[Q_{+}^{\dagger}A^{+}(x)Q_{+}]\det[Q_{-}^{\dagger}A^{-}(x)Q_{-}]\ , \quad (13)$$

where Q_{+} and Q_{-} are rectangular matrices that project out the many-electron trial wave function $|\Psi_T^n\rangle$. For zero-temperature calculations the precise form of $\rho(x)$ depends on the trial state, $|\Psi_T^n\rangle$, but in general it can be written in terms of determinants of submatrices of the $A^{\sigma}(x)$.

In order to integrate out the electron degrees of freedom one must evaluate the expectation value of individual terms of the right-hand side of Eq. (9) between the trial wave function for the zero-temperature calculation, and between elements of a complete set of states for the grand-canonical-ensemble calculation. These matrix elements can be expressed in terms of determinants of submatrices of the $A^{\sigma}(x)$. The determinants are simply the sum over all possible world lines of the electrons propagating between the initial and final states. A particular set of world lines will give a positive or negative contribution to the determinant depending on whether an even or odd number of world lines wind around each other during this propagation. Whether the positive or negative contributions to the determinant dominate depends on the values of the Hubbard-Stratonovich variables. The models under present study all have only nearest-neighbor hopping terms in the $\mathcal{H}(l)$. As a result, for small values of β there is little chance for two world lines to wind around each other, and therefore no sign problem. However, as β becomes large, there is no impediment to the world lines winding around each other. Furthermore, the Hubbard-Stratonovich fields used in studies of the Hubbard model, unlike phonon fields, have no dynamics, so there are no time derivatives which prevent them from undergoing large changes from one imaginary-time slice to another. For large β we expect that the world lines will lose knowledge of the initial state, and that the number of windings per unit imaginary-time interval will approach a constant. It then follows that the average value of the sign of $\rho(x)$ should go to zero exponentially with increasing β. Similarly the number of windings per unit time interval should grow linearly with the spatial volume, which implies that the expectation value of the sign should fall exponentially with volume. Finally we expect the sign problem to worsen as the coupling increases, since the inhomogeneities in the Hubbard-Stratonovich field then become more strongly emphasized.

In order to consider the sign in the zero-temperature calculation in more detail we make use of Eq. (9) to write

$$Z=\sum_x \langle\Psi_T^n|e^{-\Delta\tau\mathcal{H}(L)}\cdots e^{-\Delta\tau\mathcal{H}(2)}e^{-\Delta\tau\mathcal{H}(1)}|\Psi_T^n\rangle = \sum_x \rho(x)\ , \quad (14)$$

and then define $Z_{\pm}$ by

$$Z_{+}=\sum_{\rho(x)>0}\rho(x)\ , \qquad Z_{-}=-\sum_{\rho(x)<0}\rho(x)\ . \quad (15)$$

The expectation value of the sign can now be written as

$$\langle S\rangle_{\tilde{P}}=\frac{Z_{+}-Z_{-}}{Z_{+}+Z_{-}}\ . \quad (16)$$

Since Z is positive, $Z_{+}\geq Z_{-}$, and $1\geq\langle S\rangle_{\tilde{P}}\geq 0$.

There are a limited number of possibilities. If the ratio Z_{-}/Z_{+} approaches zero as β goes to infinity, then there is no sign problem. If this ratio approaches a finite limit different from unity, then $\langle S\rangle_{\tilde{P}}$ approaches a constant. This is the situation envisioned by Sorella *et al.*[1] Since Z has the eigenvalue expansion

$$Z=\sum_l e^{-\beta E_l}|\langle\psi_l|\Psi_T^n\rangle|^2\ , \quad (17)$$

if Z_{-}/Z_{+} approaches a constant, then both Z_{+} and Z_{-} must become proportional to $\exp(-\beta E_0)$ for large β. Therefore, a measurement of the β dependence of $Z_{+}+Z_{-}$, that is a measurement of Z ignoring the minus signs, would yield the ground-state energy. If this behavior were to persist over a range of parameters, then a number of ground-state properties could be calculated by differentiation of the ground-state energy.[1] However, a direct measurement of the correlation functions in which signs are ignored would lead to incorrect results. If we denote by O_{+} the average value of $O(x)$ in configurations with positive weights $\rho(x)>0$ and by O_{-} the average value in configurations with negative weights, then

$$\langle O\rangle=\frac{O_{+}Z_{+}-O_{-}Z_{-}}{Z_{+}-Z_{-}}=O_{+}+Z_{-}\frac{O_{+}-O_{-}}{Z_{+}-Z_{-}}\ . \quad (18)$$

On the other hand, if we proceed by ignoring the sign of $\rho(x)$, we obtain

$$\langle O\rangle_{\tilde{P}}=\frac{O_{+}Z_{+}+O_{-}Z_{-}}{Z_{+}Z_{+}}=O_{+}+\tfrac{1}{2}Z_{-}\frac{O_{-}-O_{+}}{Z_{+}+Z_{-}}\ . \quad (19)$$

Clearly these two expressions are equal only if $Z_{+}Z_{-}(O_{+}-O_{-})=0$. This can happen if $Z_{-}=0$, in which case there is no sign problem, or if $O_{+}=O_{-}$. There is no *a priori* reason to expect $O_{+}=O_{-}$, but since O_{+} and O_{-} are readily calculated, it would appear that one at least has an internal check on the calculation. However, when $Z_{+}-Z_{-}$ is so small as to preclude a straightforward calculation of observables according to Eq. (5), the difference $O_{+}-O_{-}$ will generally be too small to make this check reliable.

The remaining possibility is that the ratio Z_{-}/Z_{+} ap-

proaches unity as β goes to infinity. This is the result we find in our numerical studies of the Hubbard model away from half filling. In this case, as Sorella *et al.* have indicated,[1] one cannot expect to obtain exact results from calculations that ignore the sign of $\rho(x)$. We see from Eq. (18) that $\langle O \rangle$ will approach a finite limit as $Z_+ \to Z_-$ only if $O_+ \to O_-$. Under these circumstances $\langle O \rangle_{\bar{P}} \to O_+$, so $\langle O \rangle_{\bar{P}} = \langle O \rangle$ only if $(O_+ - O_-)/(Z_+ - Z_-)$ goes to zero, and in general there is no reason to expect such a result. If one assumes that the leading asymptotic behavior of Z_+ and Z_- continues to be exponential, then one sees from Eq. (17) that the expectation value of the sign will fall exponentially with β barring an accidental degeneracy. That is, both Z_+ and Z_- will have asymptotic behavior of the form $\exp(-\beta\{E_0 - \Delta\})$ with $\Delta > 0$. However, this leading behavior will cancel in $Z_+ - Z_-$ so $\langle S \rangle_{\bar{P}}$ will go to zero as $\exp(-\beta\Delta)$.

If it is possible to view calculations made ignoring the sign of $\rho(x)$ as arising from an effective Hamiltonian with ground-state wave function and energy $|\psi_0'\rangle$ and $E_0' = E_0 - \Delta$,[6] then for large β

$$\langle S \rangle_{\bar{P}} = \frac{|\langle \psi_0 | \Psi_T^n \rangle|^2}{|\langle \psi_0' | \Psi_T^n \rangle|^2} e^{-\beta(E_0 - E_0')} . \tag{20}$$

In this picture if the expectation value of the sign were to approach a finite limit at large β, then the ground-state energies of the true and effective Hamiltonians would have to be equal. The fact that the average sign is small at large β indicates that even if the ground-state energies are equal, the ground-state wave functions have different properties. The ground-state energies obey $E_0' \le E_0$. Had we ignored the sign even in the calculation of $\rho(x)$, using permanents instead of determinants, the ground-state energy would have dropped further, to the bosonic many-body ground-state energy.

An identical discussion can be made for calculations within the grand canonical ensemble. Once again we expect that the average sign to fall exponentially with increasing β. As we have previously observed,[4] the average sign depends strongly on band filling and coupling as well as on temperature. Some insight can be gained into this situation by considering the behavior of the eigenvalues of the $A^\sigma(x)$ matrices. For the two-dimensional Hubbard model with μ measured from $-U/2$, particle-hole symmetry ensures that for each eigenvalue of $A^+(x)$, λ_i, there will be a corresponding eigenvalue of $A^-(x)$, $1/\lambda_i$. Since the $A^\sigma(x)$ are real matrices, their eigenvalues are real or come in complex conjugate pairs. Finally,

$$\det A^\sigma(x) = \prod_{l=1}^{L} \det[e^{-\Delta\tau h^\sigma(x_l)}] > 0 , \tag{21}$$

so no eigenvalue can pass through zero. For zero coupling or for high temperatures all of the eigenvalues lie on the positive real axis. How then can $\rho(x)$ become negative? As the coupling is increased or the temperature decreased a pair of eigenvalues can collide and move into the complex plane. They can collide again on the negative real axis and move apart. If a negative eigenvalue passes through the point $|\lambda_i| = \exp(\mp\beta\mu)$, then $\det[I + \exp(\beta\mu) A^\pm(x)]$ will vanish. $\rho(x)$ will be negative only if an odd number of negative eigenvalues are in the range

$$\exp(-\beta\mu) \le |\lambda_i| \le \exp(\beta\mu) .$$

One sees at once that at $\mu = 0$, that is at half filling, $\rho(x)$ is positive definite.

For zero coupling $\lambda_i = \exp(-\beta\epsilon_i)$ where ϵ_i are the energy levels for the free theory. Consider, as an example, the case of a 4×4 square lattice. Then the states with energy $\pm 4t$ (t is the hopping parameter) are nondegenerate, while those with energy $\pm 2t$ are fourfold degenerate and those with energy 0 are sixfold degenerate. Once the coupling is turned on the degeneracies of the λ_i will be broken for any given Hubbard-Stratonovich configuration, but for weak to moderate coupling they will not be badly broken. It is these nearly degenerate eigenvalues that can most easily collide on the real axis and eventually become negative. If the chemical potential is fixed so that each nearly degenerate set of λ_i is either totally inside or outside the range

$$\exp(-\beta\mu) \le |\lambda_i| \le \exp(\beta\mu) ,$$

then the sign of $\rho(x)$ will not oscillate rapidly as the Hubbard-Stratonovich variables are changed. This explains the slow variation of the sign with β for fillings of 10 and 22 and the rapid variation near half filling for the Hubbard model on a 4×4 lattice. For strong coupling the eigenvalues change more rapidly in response to changes in the Hubbard-Stratonovich variable, and the sign oscillates more rapidly.

The same considerations apply to ground-state calculations. For a trial state with n_+ spin-up electrons and n_- spin-down electrons, the behavior of $\rho(x)$ at low temperatures is controlled by the n_+ largest eigenvalues of $A^+(x)$ and the n_- largest eigenvalues of $A^-(x)$, and one reaches the same conclusions regarding fluctuations in the sign. All of these conclusions are born our numerically.

III. NUMERICAL RESULTS

In this section we present numerical results for the two-dimensional Hubbard model. We write the Hamiltonian in the form

$$H = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ c_{i\sigma}) + U \sum_i (n_{i+} - \tfrac{1}{2})(n_{i-} - \tfrac{1}{2}) , \tag{22}$$

where $n_{i,\sigma} = c_{i,\sigma}^\dagger$. The factors of $\frac{1}{2}$ have been included so that the Hamiltonian is invariant under a particle-hole transformation, and half filling corresponds to $\mu = 0$. We make use of Hirsch's discrete Hubbard-Stratonovich transformation[3] to obtain

$$\mathcal{H}(l) = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ c_{i\sigma}) + \sum_i \sum_{x_l = \pm 1} x_{i,l} \lambda (n_{i+} - n_{i-}) , \tag{23}$$

with λ defined by $\cosh(\Delta\tau\lambda)=\exp(\Delta\tau U/2)$, and $x_{i,l}=\pm 1$.

Our simulations are carried out with the Monte Carlo algorithms described in details in Ref. 4. Unless otherwise specified, we present data for 4×4 lattices, and for ground-state calculations use a Hartree-Fock trial function for $|\Psi_T^n\rangle$. Where no error bars are shown, they lie inside the plotting symbol. Both β and U are measured in units of the hopping parameter t.

We begin by considering calculations of ground-state properties. In Fig. 1 we plot the expectation value of the sign as a function of β for $U=8$ with a density of 0.625 electrons per site. Sorella *et al.*[1] have calculated the expectation value of the sign for the same lattice size, coupling constant and filling. We disagree with their claim that $\langle S\rangle_{\tilde{P}}$ goes to a small, but finite, constant for large β. Indeed for our three largest values of β, 40, 48, and 64, we find $\langle S\rangle_{\tilde{P}}=0.0095\pm0.0018$, 0.0039 ± 0.0018, and -0.0006 ± 0.0015, respectively. In Fig. 2 we plot the logarithm of $\langle S\rangle_{\tilde{P}}$ as a function of β. The solid squares are the same data as in Fig. 1, while the empty squares are for a real-space trial function. The solid lines are least-squares fits to the large β portion of the data. For the Hartree-Fock wave function we use results for $\beta\geq 8.0$ and obtain a χ^2 of 4.7 for seven degrees of freedom. Our results clearly indicate that $\langle S\rangle_{\tilde{P}}$ falls exponentially with β for large β. The points for the real-space trial function have the same slope, within statistical errors, but a different intercept, than those for the Hartree-Fock trial function. In other words the trial function effects the prefactor of $\langle S\rangle_{\tilde{P}}$, but not its rate of exponential falloff, in accordance with our argument in Sec. II.

Our calculations differ from those of Sorella *et al.*[1] in several respects: we have results at twice their largest value of β, we employ a discrete rather than a continuous Hubbard-Stratonovich transformation, and we use a Monte Carlo, rather than a Langevin, algorithm. We have previously performed calculations for the grand canonical ensemble using continuous Hubbard-Stratonovich variables.[7] We find that over a range of electron densities the expectation value of the sign agrees within statistical errors with our present grand canonical calculations employing discrete Hubbard-Stratonovich variables. The calculations with continuous Hubbard-Stratonovich variables were performed with a hybrid Monte Carlo algorithm, which is quite different from our present algorithms, and therefore provides an independent check of them. We, and previously Hirsch,[3] have made extensive checks on the equilibration of the sign in Monte Carlo algorithms. We find that these algorithms have no trouble in tunneling between regions of positive

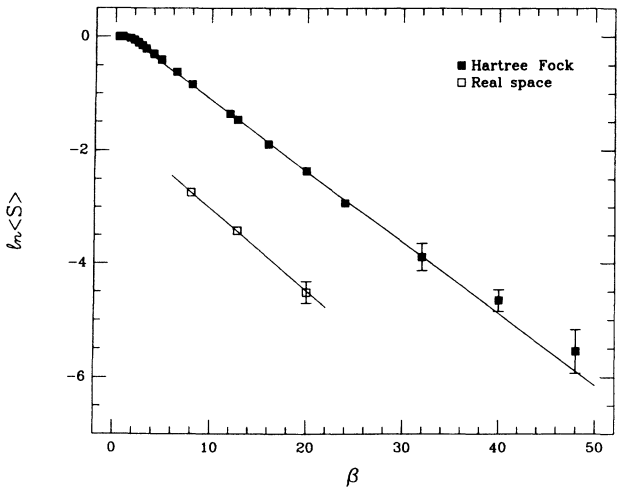

FIG. 2. The logarithm of $\langle S\rangle_{\tilde{P}}$ as a function of β on a 4×4 lattice with $U=8$ and $\langle n\rangle=0.625$. The solid squares are for a Hartree-Fock trial function and the open squares for a real-space trial function. The straight lines are least-squares fits to the large β portion of the data.

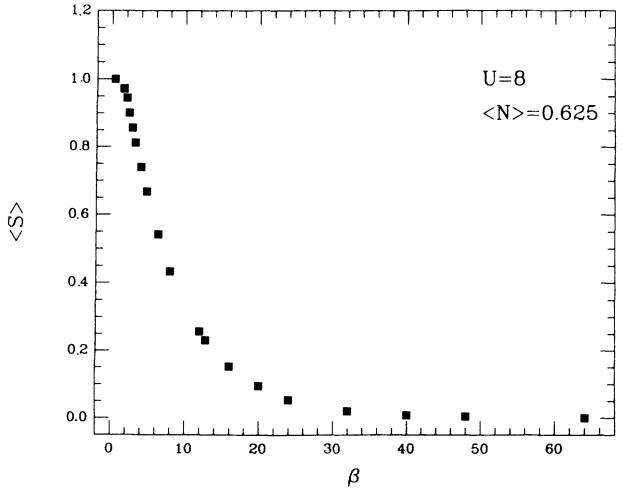

FIG. 1. The expectation value of the sign $\langle S\rangle_{\tilde{P}}$ as a function of β on a 4×4 lattice with $U=8$ and filling $\langle n\rangle=0.625$. These data are from the ground-state algorithm, as are those in Figs. 2–5.

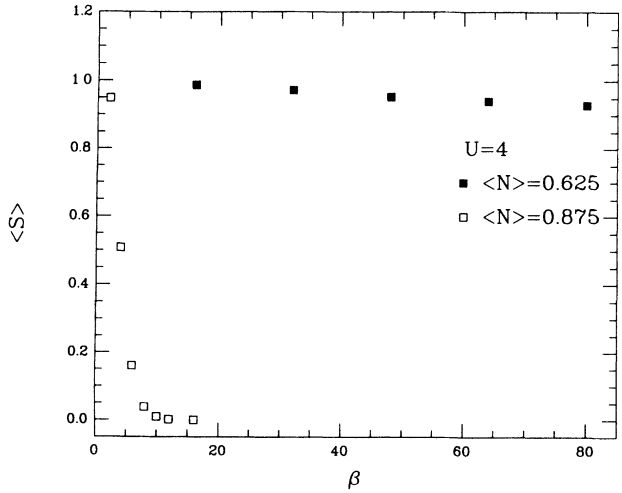

FIG. 3. The expectation value of the sign as a function of β on a 4×4 lattice with $U=4$. The solid squares are for an electron density of 0.625 and the open squares for a density of 0.875.

and negative $\rho(x)$. On the other hand, it is known that simulations employing the Langevin algorithm can go out of equilibrium when crossing nodal surfaces.[8]

In Fig. 3 we plot $\langle S \rangle_{\bar{P}}$ as a function of β at $U=4$ for the ground-state algorithm. The solid squares are for an electron density of 0.625 and the open squares for a density of 0.875. Figures 4 and 5 show semilog plots of the same data. Again the straight lines are least-square fits to the large β portion of the data. We see that $\langle S \rangle_{\bar{P}}$ falls exponentially with β for both fillings, but with very different decay rates. The variation in decay rates with filling and coupling are in accordance with our discussion in the preceding section.

In Fig. 6 we again plot the logarithm of $\langle S \rangle_{\bar{P}}$ as a function of β for $U=8$ with a filling of 0.625. The solid squares are the ground-state algorithm data of Figs. 1 and 2. The open squares are from a grand-canonical-ensemble calculation. The straight lines are again least-squares fits to the high β portion of the data. The slopes of the two lines agree within statistical errors, but the line from the grand-canonical-ensemble calculation has an intercept that lies somewhat below that from the ground-state calculation. We believe that the smaller value of the sign in the grand-canonical-ensemble simulation is due to electron number fluctuations. Finally we note that we have previously presented data showing that for the grand-canonical ensemble the sign falls with increasing spatial volume.[4]

In all calculations that we have preformed to date, we find strong evidence that the expectation value of the sign falls exponentially with β. This does not mean that one cannot obtained useful information about the ground-state energy. As Sorella *et al.* have pointed out,[1] it is straightforward to calculate the β dependence of $Z_+ + Z_-$, because no fluctuating signs are involved. This calculation yields the quantity $E_0' = E_0 - \Delta$. A measurement of the β dependence of $\langle S \rangle_{\bar{P}}$ yields Δ, and therefore E_0. For example, for $U=8$ with a filling of 0.625 and $\Delta\tau = 0.1$ we find $E_0' = E_0 - \Delta = -17.75 \pm 0.06$. Our least-squares fit to the logarithm of $\langle S \rangle_{\bar{P}}$ yields a correction, $\Delta = 0.126 \pm 0.002$. Δ varies significantly with filling and coupling, but in all cases that we have studied to date, it is a small compared to E_0. It should be possible to significantly reduce the error bars on E_0', so that at least on small lattices this approach can be used to obtain accurate measurements of the ground-state energy as a function of filling and coupling. Whether this procedure or a straightforward measurement including the signs produces superior results is likely to depend on the relative size of Δ and the gap to the first excited state.

Our results suggests that it may be possible to perform

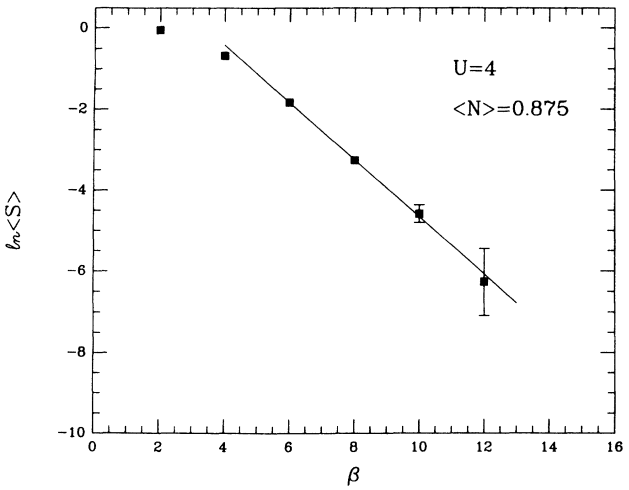

FIG. 5. The logarithm of $\langle S \rangle_{\bar{P}}$ as a function of β on a 4×4 lattice with $U=4$ and $\langle n \rangle = 0.875$. The straight line is a least-squares fit to the large β portion of the data.

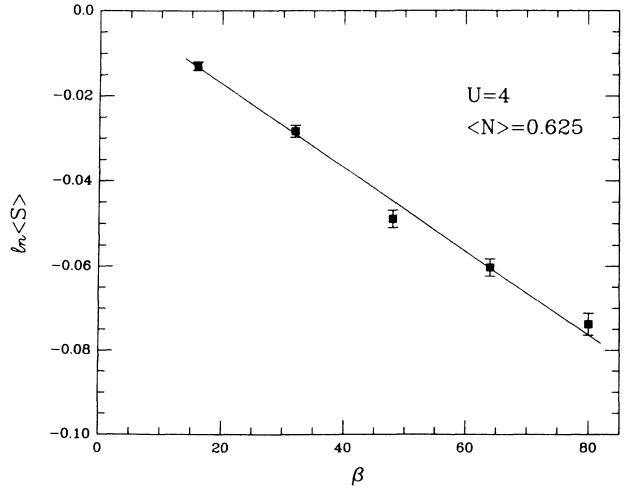

FIG. 4. The logarithm of $\langle S \rangle_{\bar{P}}$ as a function of β on a 4×4 lattice with $U=4$ and $\langle n \rangle = 0.625$. The straight line is a least-squares fit to the large β portion of the data.

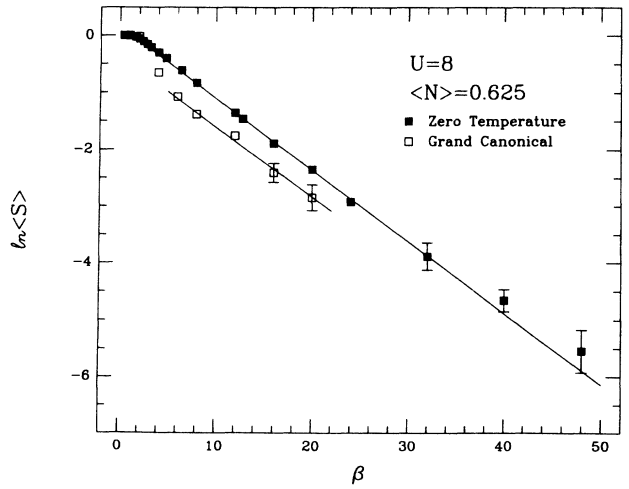

FIG. 6. The logarithm of $\langle S \rangle_{\bar{P}}$ as a function of β on a 4×4 lattice with $U=8$ and $\langle n \rangle = 0.625$. The solid squares are data from the ground-state algorithm and the open squares from the grand-canonical-ensemble algorithm. The straight lines are least-squares fits to the large β portions of the data. The slopes of these lines agree with statistical errors.

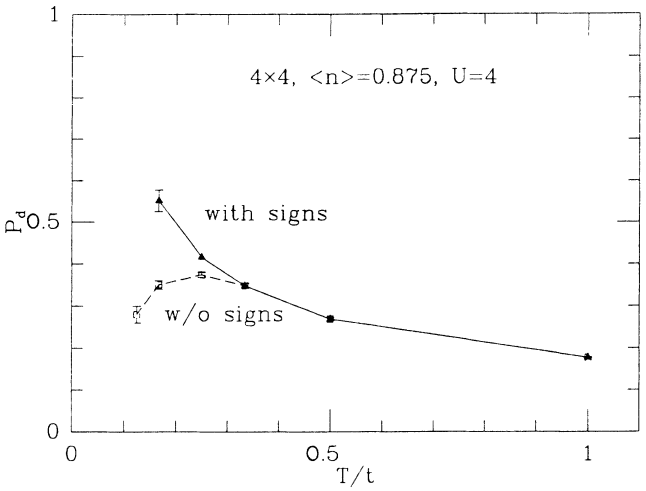

FIG. 7. The d-wave pairing susceptibility, P_d as a function of temperature on a 4×4 lattice with $U=4$ and $\langle n\rangle=0.875$. The solid triangles (solid line) are for a correct Monte Carlo calculation, and the open squares (dashed line) are for the same configurations but neglecting the sign of the fermion determinant.

calculations of ground-state properties of other quantities, but not with the accuracy that can be achieved for the energy. The small value of Δ is an indication that the neglect of signs yields a good first approximation for the energy. We have performed ground-state calculations of a variety a quantities, neglecting the sign, on 2×2 lattices with an electron density of 0.75. For example, for the structure function $S(\pi,\pi)$ we find 0.91 ± 0.02 and 0.93 ± 0.03 for $U=4$ and 8, respectively. Exact calculations yield 0.906 and 0.982 for these quantities. For the potential energy at these two couplings we find 1.13 ± 0.01 and 1.25 ± 0.05 as compared to exact results of 1.198 and 1.362. Similar calculations within the grand-canonical ensemble do not produce quite such good results. These calculations indicate that, at least on the small lattices, the quantity O_+ is a good first approximation to $\langle O\rangle$. This quantity can be obtained with very good statistics, since it does not involve minus signs. We see from Eq. (18) that the correction term needed to make an exact calculation is

$$Z_-\frac{O_+-O_-}{Z_+-Z_-}=\tfrac{1}{2}(O_+-O_-)\left[\frac{1}{\langle S\rangle_{\bar{P}}}-1\right]. \quad (24)$$

As long as this term remains a small correction to O_+, the fact that it is noisy will not be too serious. Notice that the correction term vanishes when $\langle S\rangle_{\bar{P}}=1$. In some instances it also becomes small when $\langle S\rangle_{\bar{P}}\to0$. For example, on our standard 4×4 lattice with $U=8$ and a density of 0.625, we find the $S(\pi,\pi)_+$ has the constant value 0.775 ± 0.008 in the entire range $12\le\beta\le24$. For this range of β the quantity $S(\pi,\pi)_+-S(\pi,\pi)_-$ is zero within statistical errors which are of order ±0.02. To make a precise determination of the correction term of Eq. (24) requires a high-statistics calculation of the quantity $\frac{1}{2}(O_+-O_-)$. Whether this approach will lead to a useful calculational method is under investigation.

It should be emphasized that the neglect of the sign of the fermion determinant is an uncontrolled approximation, and can lead to misleading results if the correction terms are not included. As an example, we show in Fig. 7 the d-wave pairing susceptibility P_d as a function of temperature on a 4×4 lattice for $U=4$ and $\langle n\rangle=0.875$. Recall that the interesting physical question is whether P_d diverges at low temperature.

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