

Algorithm for the simulation of many-electron systems at low temperatures

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(Received 18 July 1988)

We present a new algorithm for the numerical simulation of many-electron systems, which is particularly effective for the study of two-dimensional models at low temperatures. We present results for the two-dimensional Hubbard model on lattices as large as 8×8 and inverse temperatures as large as $\beta = 10$. As the temperature is lowered, we find a continuous rise in the d -wave pairing susceptibility, indicating the possibility of a phase transition to a superconducting state.

Numerical simulations potentially provide a powerful tool for the study of strongly interacting electronic systems; however, it has proven difficult to carry out such simulations at low temperatures. This has made it difficult to study a number of systems, such as two-dimensional models of high-temperature superconductors, for temperatures of physical interest. In this paper we present a new algorithm which we believe has great promise for the study of such systems.

Two major problems arise in the simulation of many-electron systems at low temperatures. Both are related to the fact that the integrands of the path integral being evaluated are proportional to the determinants of fermion matrices. First, in the course of the simulation it is necessary to repeatedly calculate the inverses of the fermion matrices, which become progressively more ill conditioned as the temperature is lowered.^{1,2} Second, at low temperatures the fermion determinants can change sign.³ On the surfaces where they vanish the probability function used in the simulation also vanishes. It is essential that the algorithm allow for efficient tunneling across such surfaces, or else regions of configuration space with opposite signs of the determinants will not come to equilibrium with each other.²⁻⁴ The algorithm we introduce here incorporates advances in dealing with both of these problems.

Our starting point is the partition function

$$Z = \text{tr} e^{-\beta H}, \quad (1)$$

where β is the inverse temperature and H is the Hamiltonian. We shall illustrate our approach by studying the two-dimensional Hubbard model, although our algorithm can be straightforwardly applied to a wide variety of electron and electron-phonon systems in two-dimensions. The Hamiltonian for the Hubbard model is

$$H = -t \sum_{\langle ij \rangle} \sum_{\sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}) + \sum_i [U(n_{i+} - \frac{1}{2})(n_{i-} - \frac{1}{2}) - \mu(n_{i+} + n_{i-})]. \quad (2)$$

Here $c_{i\sigma}^{\dagger}$ and $c_{i\sigma}$ are the creation and annihilation operators for an electron on the i th lattice site with z component of spin σ , $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$, and $\langle ij \rangle$ specifies a pair of nearest-neighbor lattice sites. The first term in the Hamiltonian represents the kinetic energy of the electrons, the second term the on-site Coulomb interaction, and the third the chemical potential.

In order to carry out a numerical calculation, we must integrate out the electron degrees of freedom in Eq. (1), and express the partition function as a path integral over a set of bosonic coordinates. To this end we divide the interval 0 to β into L imaginary-time slices of width $\Delta\tau$, and separate the kinetic energy and interaction terms using the Trotter approximation. At this point we deviate from standard practice by introducing at each lattice point i and time slice l a complex Hubbard-Stratanovitch transformation:

$$\begin{aligned} \exp[-\Delta\tau U(n_{i+} - \frac{1}{2})(n_{i-} - \frac{1}{2})] &= \exp\{-\frac{1}{2}\Delta\tau U[n_{i+}(e^{2i\theta} - 1) + n_{i-}(e^{-2i\theta} - 1) + \frac{1}{2}]\} \\ &\times \left[\frac{\Delta\tau}{\pi} \right]^{1/2} \int_{-\infty}^{+\infty} dx_{i,l} \exp\{-\Delta\tau[x_{i,l}^2 + (2U)^{1/2}x_{i,l}(n_{i+}e^{i\theta} - n_{i-}e^{-i\theta})]\}. \end{aligned} \quad (3)$$

Equation (3) with $\theta = 0$ has been used extensively in studies of the Hubbard model.⁵ As we shall see, the use of small, nonzero values of θ can be extremely useful for promoting efficient tunneling in configuration space.

Making use of Eq. (3), the partition function can be written in the form

$$\begin{aligned}
Z &= \int_{-\infty}^{+\infty} \prod_{i,l} dx_{i,l} \exp \left[-\Delta\tau \sum_{i,l} x_{i,l}^2 \right] \text{tr} \left[\prod_{l,\sigma} \exp \left[-\Delta\tau \sum_{i,j} c_{i,\sigma}^\dagger h_{i,j}^\sigma(l) c_{j,\sigma} \right] \right] \\
&= \int_{-\infty}^{+\infty} \prod_{i,l} dx_{i,l} \exp \left[-\Delta\tau \sum_{i,l} x_{i,l}^2 \right] \det M_+ \det M_- .
\end{aligned} \tag{4}$$

Here $h^\sigma(l)$ is a matrix with dimension equal to the number of spatial lattice sites. It is the Hamiltonian for a single electron with z component of spin σ propagating through an external field associated with the x field on the l th time slice.

In Monte Carlo simulation of the Hubbard and related models, it has been standard practice to use $\theta=0$, and to write the fermion matrix in the form¹

$$M_\sigma = I + B_L^\sigma B_{L-1}^\sigma \cdots B_1^\sigma , \tag{5}$$

where $B_l^\sigma = \exp[-\Delta\tau h^\sigma(l)]$ and I is the unit matrix. The matrix elements of M_σ increase exponentially with β , so as the temperature is decreased it becomes increasingly difficult to calculate the determinant and inverse of M_σ . This problem can be alleviated significantly by replacing the right-hand side of Eq. (5) with a matrix having the *same determinant* but twice the dimension. We write

$$M'_\sigma = \begin{pmatrix} b_2^\sigma & 0 \\ 0 & b_4^\sigma \end{pmatrix} \begin{pmatrix} b_1^\sigma & -b_2^{\sigma-1} \\ b_4^{\sigma-1} & b_3^\sigma \end{pmatrix} . \tag{6}$$

Here

$$b_\alpha^\sigma = B_{\alpha L/4}^\sigma B_{\alpha L/4-1}^\sigma \cdots B_{(\alpha-1)L/4+1}^\sigma .$$

Note that $M_\sigma = I + b_4^\sigma b_3^\sigma b_2^\sigma b_1^\sigma$. Although the two forms of the fermion matrices have the same physical content, the matrix elements of b_α^σ are roughly the same size as those of M_σ at four times the temperature. Furthermore, the determinant of the first matrix in (6) is trivially evaluated. Hence, it is possible to calculate the determinant and inverse of M'_σ by Gaussian elimination at significantly lower temperatures without encountering problems associated with roundoff errors. With standard algorithms M_σ can be used for the two-dimensional Hubbard model with $U=4$ and $t=1$ only up to $\beta=4$,⁶ while with M'_σ and the present algorithm one can go to $\beta=10$. It appears that one can go to even lower temperatures by further enlarging the dimension of the fermion matrix in analogy with Eq. (6).⁷

We now address the question of tunneling between regions where the sign of the determinants changes. For $\theta=0$ the individual fermion determinants are real, but not positive definite.³ The product of the spin up and spin down determinants is non-negative for zero chemical potential, but not otherwise. For $\theta \neq 0$ the determinants are complex, and configuration space is no longer divided into disjoint regions by surfaces along which they vanish. In order to develop a probability distribution function for the simulation we define a real effective action S_θ through

$$\exp[-S_\theta(x)] = \exp \left[-\Delta\tau \sum_{i,l} x_{i,l}^2 \right] |\det M'_+ \det M'_-| . \tag{7}$$

Because we shall use molecular dynamics, that is,

Hamilton's equations, as part of our updating scheme, we introduce the effective Hamiltonian

$$\mathcal{H}_\theta(p,x) = \sum_{i,l} p_{i,l}^2 + S_\theta . \tag{8}$$

The $p_{i,l}$ are to be interpreted as momenta conjugate to $x_{i,l}$. If we generate a sequence of field configurations distributed as $\exp[-\mathcal{H}_\theta(p,x)]$, then the expectation value of a physical observable A can be obtained by averaging within this distribution,

$$\langle A \rangle = \frac{\langle A P_\theta \rangle_{\mathcal{H}_\theta}}{\langle P_\theta \rangle_{\mathcal{H}_\theta}} , \tag{9}$$

where P_θ is the product of the phases of the spin-up and spin-down determinants.

We are now in a position to describe the algorithm. The presence of the fermion determinants makes it quite time consuming to compute the effective action or changes in it. To minimize this calculation we suggest changes in all components of the x and p fields simultaneously, and then accept or reject the entire change according to the Metropolis algorithm.⁸ If we were to suggest the changes randomly, the acceptance probability would be prohibitively small. Instead, we suggest changes in the fields by integrating Hamilton's equations for \mathcal{H}_θ with $\theta \neq 0$.⁹ We do not use $\theta=0$ in this integration because surfaces in configuration space along which either of the fermion determinants vanished would give rise to infinite potential barriers which could not be crossed.^{2,4} Thus the system would not be able to tunnel between regions with different signs of the determinants. For $\theta \neq 0$ the fermion determinants become complex. The imaginary parts of the determinants make the barriers finite, and the system can move smoothly between such regions.

Tunneling across the barriers is facilitated by making θ large. On the other hand, we have found that the expectation value of P_θ is a maximum, and statistical fluctuations in measured quantities a minimum, for $\theta=0$. In order to maximize the performance of the algorithm we carry out the simulation, in particular the acceptance (rejection) steps and the measurements, at $\theta=0$. However, we suggest new values of the x and p fields for the Metropolis steps by integrating Hamilton's equations for \mathcal{H}_θ with $\theta \neq 0$. It should be emphasized that in suggesting changes in x and p one need only ensure that all regions of phase space are accessible and that detailed balance is satisfied. The latter is achieved by using the leap from method to perform the integration of Hamilton's equations.^{2,9} The parameter θ is at our disposal. By increasing it one tends to increase the tunneling rate between regions of different sign, while by decreasing it one tends to increase the acceptance probability and thereby move through configuration space more rapidly. In our calculations we have found that $\theta \approx 0.2$ gives both good

TABLE I. Average value of the sign of the spin-up determinant $\langle S_+ \rangle_{\mathcal{H}_0}$, and the product of the signs of the spin-up and -down determinants, $\langle S_+ S_- \rangle_{\mathcal{H}_0} = \langle P_0 \rangle_{\mathcal{H}_0}$, as a function of the inverse temperature β , lattice size, and band filling $\langle n \rangle$. In all cases $t=1$ and $U=4$. The numbers in parentheses are statistical errors in the last digit shown. In the last four entries, the chemical potential was set to $\mu=-1.0$. The resulting band fillings, which varied slowly with temperature are shown. The filling in the last entry is estimated, as the small value of $\langle S_+ S_- \rangle_{\mathcal{H}_0}$ made calculation of $\langle n \rangle$ or any other observable infeasible. Otherwise, when no errors are given, the result is exact, or the error is in a decimal place not shown.

β	Lattice	$\langle n \rangle$	$\langle S_+ \rangle_{\mathcal{H}_0}$	$\langle S_+ S_- \rangle_{\mathcal{H}_0}$
2	4×4	1.00	1.00	1.00
4	4×4	1.00	0.94	1.00
4	8×8	1.00	0.96(2)	1.00
6	2×2	1.00	0.85	1.00
6	4×4	1.00	0.69(5)	1.00
6	8×8	1.00	0.11(9)	1.00
8	4×4	1.00	0.36(5)	1.00
10	4×4	1.00	0.42(4)	1.00
4	4×4	0.85(1)	0.93(1)	0.90(2)
6	4×4	0.83(3)	0.56(2)	0.34(2)
6	6×6	0.82(7)	0.39(3)	0.19(4)
8	4×4	0.83	0.3(1)	0.07(6)

acceptance rates (typically about 50%) and rapid tunneling. In order to allow for large changes in \mathcal{H}_0 we precede each updating step which we have just discussed with a heat bath updating of the p field. That is, we replace each element of p with random numbers distributed as $\exp(-p_{i,l}^2)$.

The Metropolis acceptance (rejection) step removes the errors normally associated with integrating Hamilton's equations with a finite step size Δt .⁹ The only effect of a large Δt is a reduced acceptance rate. We have found that one can use quite large step sizes ($\Delta t=0.3-0.7$ in the results presented) and still obtain satisfactory acceptance rates.

In Table I we present data for the average value of the sign of an individual determinant, $\langle S_+ \rangle$, and the average of the product of the signs of the two determinants, $\langle S_+ S_- \rangle_{\mathcal{H}_0} = \langle P_0 \rangle_{\mathcal{H}_0}$, with $U=4$ and $1 \leq \beta \leq 10$ for both $\mu=0$ and $\mu=-1$. The tunneling rate is rapid enough to provide excellent equilibrium of P_0 . When $\langle S_+ S_- \rangle_{\mathcal{H}_0}$ is close to zero, even modest statistical errors in the numerator and denominator of Eq. (9) give rise to large errors in $\langle A \rangle$. It is clear from the $\mu=-1$ results that at sufficiently low temperatures, there will be values of the chemical potential for which simulations will be difficult. However, it is also clear that the present algorithm will allow us to explore a very interesting region of temperatures.

In Fig. 1 we show results for the antiferromagnetic correlation function $S(\pi, \pi)$, as a function of temperature for $U=4$ and $\mu=0$. In order to check our algorithm we have diagonalized the Hamiltonian for the two-dimensional Hubbard model on a 2×2 lattice. The exact

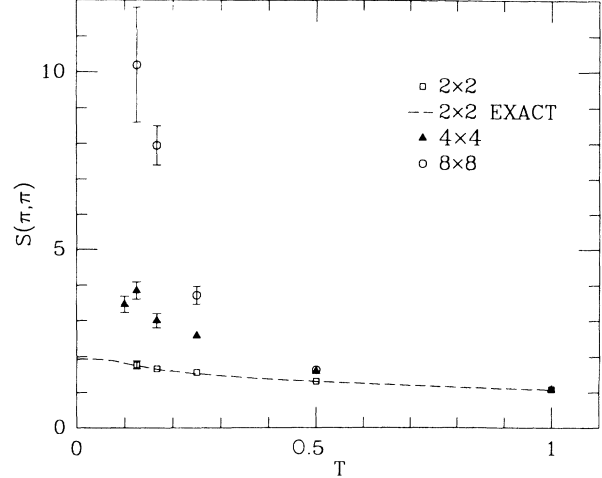


FIG. 1. Antiferromagnetic correlation function, $S(\pi, \pi)$, as a function of temperature for the half-filled Hubbard model. The dashed line is the result of an exact diagonalization of the Hamiltonian for the 2×2 lattice. The statistical error is smaller than the plotting symbols where not shown.

results are shown by the dashed line in Fig. 1, and the corresponding Monte Carlo data by open squares. On the same figure we show results for 4×4 and 8×8 lattices. Figure 2 shows data for the d -wave superconducting susceptibility, \mathcal{P}_d , for $U=4$ and $\mu=-1$. We again show both exact and Monte Carlo results for 2×2 lattices, as well as Monte Carlo results for 4×4, 6×6, and 8×8 lattices. Note that in all cases \mathcal{P}_d increases monotonically as the temperature is lowered, indicating the possibility of a phase transition to a superconducting phase at sufficiently low temperature.

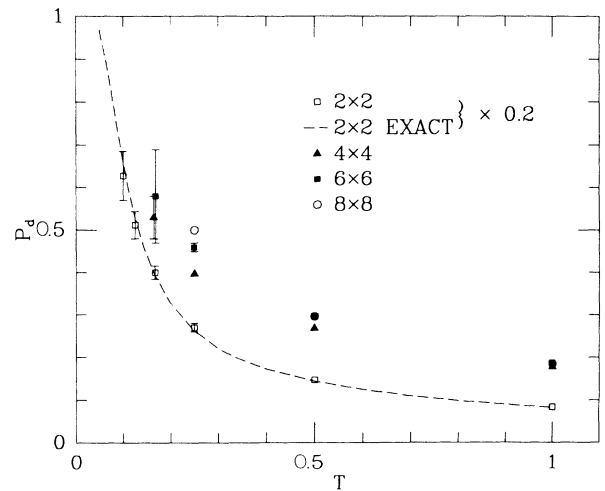


FIG. 2. The d -wave pairing susceptibility \mathcal{P}_d , as a function of temperature. The chemical potential was set to $\mu=-1.0$, which resulted in a band filling, $\langle n \rangle$ that varied slowly with temperature, with $\langle n \rangle \approx 0.84$ for the 4×4, 6×6, and 8×8 systems. The dashed line is as in Fig. 1; all results for the 2×2 system have been rescaled by a factor of 0.2 to fit on the figure. The 6×6 and 8×8 points coincide for $T=0.5, 1.0$.

Our results for \mathcal{P}_d on the 4×4 lattice are larger than those obtained by Hirsch and Lin⁶ for $\beta \geq 4.0$. They find a dip in \mathcal{P}_d for this temperature range, while we find that \mathcal{P}_d continues to rise. We have compared our results for \mathcal{P}_d with those of Hirsch and Lin for a variety of temperatures and lattice sizes. In all cases that we have checked, we find agreement with their results obtained with the older Monte Carlo algorithm.¹ Our only disagreement is with the two lowest temperature points obtained with their new "impurity algorithm."^{6,10}

These preliminary results shown that this algorithm will allow us to simulate the two-dimensional Hubbard model on significantly larger spatial and temporal lattices than has previously been possible. The computer time needed for the present algorithm grows roughly as $aN^3 + bN^2L$, where N is the number of spatial lattice points, L is the number of time slices, and a and b are constants. The first term arises from the computation of the inverse and determinant of the $2N \times 2N$ fermion matrices by Gaussian elimination, and the second term from the multiplication of L sparse $N \times N$ matrices to form the elements of M'_σ .

We believe that the algorithm that we have just described has great potential for the study of two-dimensional models of interest in connection with high-

temperature superconductivity. We are presently applying it to the two-dimensional Hubbard model, and copper-oxygen lattices. In its present form the algorithm does not appear to be applicable to three-dimensional systems, since the computer time grows so rapidly with the spatial volume. However, by combining the complex Hubbard-Stratanovitch transformation with the hybrid-molecular dynamics approach² it may be possible to work on large spatial lattices at low temperatures. The form of the fermion matrix given in Eq. (6) may also extend the range of applicability of the standard Monte Carlo approach.^{1,3} We plan to investigate both of these possibilities.

ACKNOWLEDGMENTS

We wish to thank J. E. Hirsch and D. J. Scalapino for helpful conversations. The numerical work reported in this paper was done on the Cray-XMP at the San Diego Supercomputer Center (SDSC). We wish to thank SDSC for its support. This research was supported in part by Department of Energy Grant No. DE-FG03-88ER45197 and by National Science Foundation Grant No. DMR 86-12860.

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