Monte Carlo study of a two-dimensional spin-polarized fermion lattice gas

D. J. Scalapino and R. L. Sugar
Department of Physics and Institute for Theoretical Physics, University of California, Santa Barbara, California 93106

W. D. Toussaint
Department of Physics, University of California, San Diego, La Jolla, California 92093

(Received 13 December 1983)

A model of spin-polarized fermions hopping on a two-dimensional lattice with a near-neighbor repulsive interaction is simulated with the use of Monte Carlo methods. This system exhibits an Ising-like order-disorder phase transition as the temperature is lowered. Results for the structure factor, staggered susceptibility, and order parameter are obtained, and finite-size scaling on lattices of 4×4, 6×6, and 8×8 is used to estimate T_c and test the nature of the phase transition.

Properties of two-dimensional spin-polarized quantum lattice gases are of current interest. Adsorbed submonolayers of spin-polarized $^3He_\downarrow$ and $D_\downarrow$ form examples of fermion lattice gases. Here we present results of a Monte Carlo simulation of a half-filled two-dimensional spin-polarized fermion lattice gas interacting via a near-neighbor repulsive interaction. As the temperature of the system is lowered, the staggered-site susceptibility increases, and below a transition temperature long-range order is established. We have calculated the structure factor $S(\vec{q})$, the staggered susceptibility, and the order parameter. This example indicates how recently developed stochastic methods[1] for treating interacting many-fermion systems can be used to obtain insight into the physical properties of systems in which both band-structure effects and correlations are important.

The model we study has the form

$$H=\sum_{(ij)}[-t(c_i^\dagger c_j+c_j^\dagger c_i)+V(n_i-\tfrac{1}{2})(n_j-\tfrac{1}{2})] \ , \quad (1)$$

with $i=(i_x,i_y)$ and $j=(j_x,j_y)$ the nearest-neighbor points on a square, two-dimensional spatial lattice. Here t is the single fermion transfer integral between sites and V is the strength of the nearest-neighbor repulsion. c_i creates and $c_i^\dagger$ destroys a fermion on the ith site, and n_i is the occupation number, $c_i^\dagger c_i$. We are interested in the one-half-filled band case so that Eq. (1) is written in a particle-hole symmetric form.

The ratio V/t determines whether the lattice gas is basically classical or quantum. When V/t is large compared with 1, the system approaches the classical Onsager limit. In this case an order-disorder transition occurs at a temperature $T_c=0.56$ V. In the low-temperature ordered state of the half-filled lattice, the near neighbors of an occupied site are empty, and there are two possible ordered states. We have checked our simulations for $V/t\gg1$ and find the usual Ising behavior. When V/t is less than or of order 1, quantum effects become important. In order to understand the quantum limit, it is useful to consider the nesting properties of the Fermi surface of the noninteracting $V=0$ system. In the case of a half-filled lattice, the fermions fill the lowest $N/2$ eigenstates $E_{\vec{k}}=-2t(\cos k_x+\cos k_y)$ leading to a square Fermi surface rotated by 45° with respect to the k_x-k_y axes. Particle-hole transitions with momentum $2\vec{k}_F=(\pi,\pi)$ give a perfect nesting of the Fermi surface so that mean-field theory predicts that the interacting system will undergo a second-order phase transition to a density wave state with a period of $(2k_F)^{-1}$. In the following we have taken $t=V=1$ and carried out simulations on 4×4, 6×6, and 8×8 lattices.[2]

At finite temperatures the average value of an operator O is given by

$$\langle O\rangle=\mathrm{Tr}(Oe^{-\beta H})/\mathrm{Tr}(e^{-\beta H}) \ . \quad (2)$$

In order to construct a representation of Eq. (2) that is suitable for numerical simulation, we divide the imaginary-time interval $0\leq\tau\leq\beta$ into M equal subintervals of width $\Delta\tau$, so that $M\Delta\tau=\beta$. We then make use of a discrete Hubbard-Stratonovich transformation recently introduced by Hirsch:[3]

$$\exp[-\Delta\tau V(n_i-\tfrac{1}{2})(n_j-\tfrac{1}{2})]=e^{-\Delta\tau V/4}\tfrac{1}{2}\sum_{S_{ij}=\pm1}\exp[\Delta\tau J(n_i-n_j)S_{ij}] \ , \quad (3)$$

with $\cosh(\Delta\tau J)=e^{\Delta\tau V/2}$.

Using Eq. (3) we write the partition function Z in the form

$$Z=\mathrm{Tr}e^{-\beta H}=\mathrm{Tr}\sum_{S_{ij}(\tau_l)=\pm1}T\exp\left[-\Delta\tau\sum_l\sum_{ij}[-t(c_i^\dagger c_j+c_j^\dagger c_i)+JS_{ij}(\tau_l)(n_i-n_j)]\right] \ , \quad (4)$$

with a similar expression for the numerator of Eq. (2). Here $S_{ij}(\tau_l)$ is a spin variable which one can think of as being associated with the lattice bond between the ith and jth site on the lth time slice. T indicates a τ-ordered product. Equation (4) is exact only in the limit $\Delta\tau\to0$ with $\Delta\tau M=\beta$ fixed. In our numerical calculations we keep $\Delta\tau$ finite, but small enough so as not to introduce errors larger than our statistical ones.

Since the effective Hamiltonian of Eq. (4) is quadratic in the fermion creation and annihilation operators, the trace over fermion degrees of freedom can be performed analytically yielding

$$Z=\sum_{S_{ij}(\tau_l)=\pm 1}\det\left[I+T\exp\left[-\Delta\tau\sum_l h(\tau_l)\right]\right] , \tag{5}$$

with $h(\tau_l)$ the Hamiltonian matrix for a single particle which can hop to near-neighbor points on the lattice with matrix element $-t$ and which feels a potential on the ith lattice site of

$$J[S_{\vec{i},\vec{i}+\hat{x}}(\tau_l)+S_{\vec{i},\vec{i}+\hat{y}}(\tau_l)-S_{\vec{i},\vec{i}-\hat{x}}(\tau_l) \times S_{\vec{i},\vec{i}-\hat{y}}(\tau_l)] .$$

Following the procedure discussed in Ref. 1, a set of spin configurations are generated such that the probability of the occurrence of a given configuration is proportional to the determinant of Eq. (5). It is straightforward to solve the single-particle problem of an electron moving in a potential determined by a particular spin configuration and hence to compute various physical quantities for that configuration. Then by averaging over the set of spin configurations, the effects of the interaction are taken into account just as in the usual continuous Hubbard-Stratonovich procedure.

Figure 1 shows the density-density x-ray structure factor

$$-S(\vec{q})=\sum_l e^{i\vec{q}\cdot\vec{l}}\langle n_{\vec{l}+\vec{l}}n_{\vec{l}}\rangle \tag{6}$$

on an 8×8 lattice for $T=0.667$. A peak in $S(\vec{q})$ at $(q_x,q_y)=(\pi,\pi)$ is clearly evident. Figure 2 shows the growth of this peak, $S(\pi,\pi)$, as the temperature is lowered for $L\times L$ lattices with $L=4$, 6, and 8. In a bulk system we expect that below a critical temperature T_c, $S(q)$ will exhibit a Bragg peak at (π,π), corresponding to the formation of a density wave phase with an amplitude proportional to the square of the order parameter

$$\langle O\rangle=\frac{1}{L^2}\sum_l(-1)^{l_x+l_y}\langle n_{\vec{l}+\vec{l}}-\tfrac{1}{2}\rangle . \tag{7}$$

Here L^2 is the total number of sites.

Another quantity of physical interest is the response α to a static staggered potential. This susceptibility is given in terms of the order parameter, order-parameter correlation function

$$\alpha=L^2\int_0^\beta\langle O(\tau)O(0)\rangle\,d\tau , \tag{8}$$

with $O(\tau)=e^{H\tau}Oe^{-H\tau}$. Figure 3 shows α versus temperature for lattices of linear dimension $L=4$ and 6. Note that in Eq. (8) we have not taken the usual definition of α in which $L^2\langle O\rangle^2\beta$ is subtracted.

These results for the structure factor S and the staggered

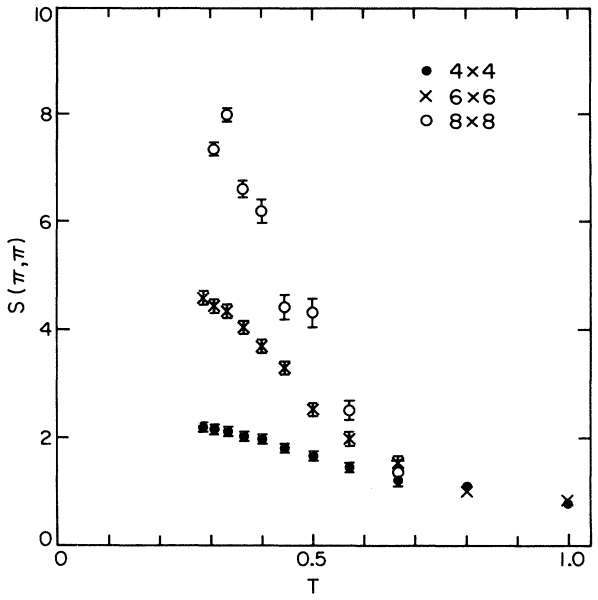

FIG. 2. Peak in the structure factor $S(\pi,\pi)$ vs temperature T for three different lattice sizes $L=4$, 6, and 8.

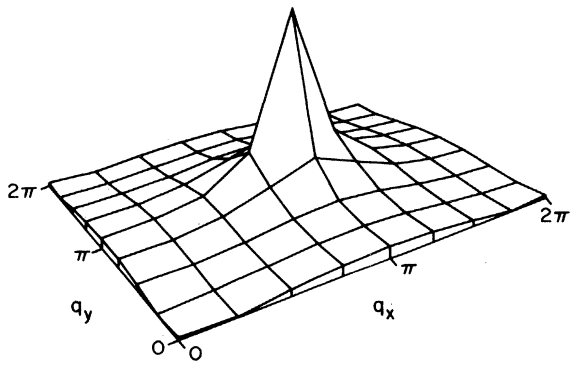

FIG. 1. Structure factor $S(q_x,q_y)$ for $T=0.667$ on an 8×8 lattice.

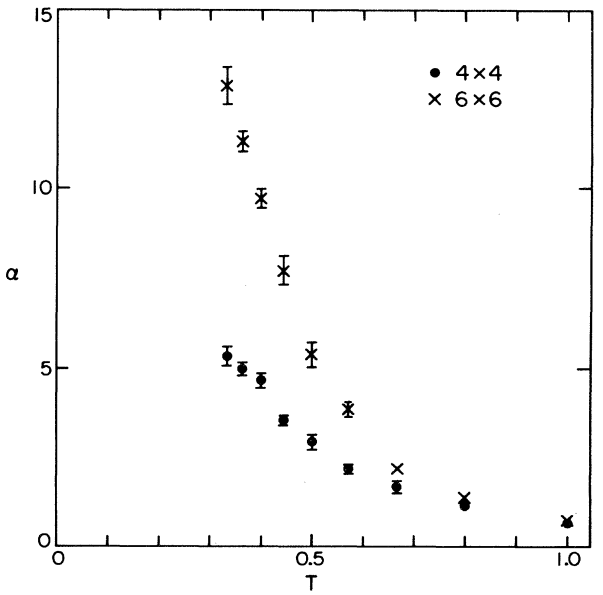

FIG. 3. Staggered susceptibility $\alpha(T)$ vs temperature for lattices with $L=4$ and 6.

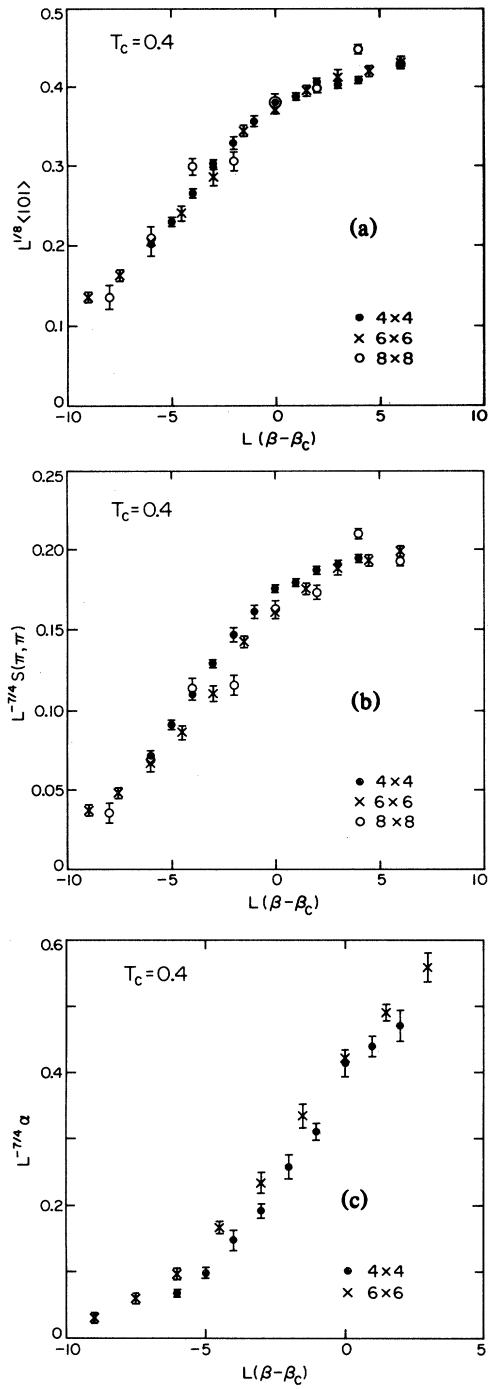

FIG. 4. Scaling plots based upon two-dimensional Ising critical indices and $T_c = 0.4$ for (a) the magnitude of the order parameter $\langle|O|\rangle$, (b) the peak in the structure factor $S(\pi,\pi)$, and (c) the staggered polarizability. In these plots $\beta = 1/T$.

susceptibility α suggest that this system undergoes a phase transition to a density wave state characterized by $\vec{q} = (\pi,\pi)$ reflecting the $2p_F$ nesting of the Fermi surface. This is just the quantum limit of the classical Ising transition. As noted before, when the transfer integral t in Eq. (1) vanishes, our model reduces to a two-dimensional (2D) Ising model with $n_l - \frac{1}{2}$ equal to an effective spin S_l^z. For small values of t, an expansion in the hopping introduces only finite-range effective spin couplings, and hence, for weak t, the system remains in the 2D Ising universality class. Therefore, barring a crossover to another type of fixed point when t becomes comparable with V, the transition should be characterized by the 2D Ising indices. Using finite-size scaling we can explore the consistency of this and obtain an estimate of T_c.

According to the ideas of finite-size scaling,[4] if for a bulk system near T_c a quantity $F(\beta) \approx |\beta - \beta_c|^{-P}$, then in a large but finite system this quantity will vary as

$$F_L(\beta) \approx L^{P/\nu} G[(\beta-\beta_c)L^{\nu}] \ . \tag{9}$$

Here L is the lattice size, ν is the correlation length exponent which is 1 for the 2D Ising model, and G is a universal scaling function. For the order parameter $\langle O\rangle$ we have taken $P = \frac{1}{8}$, the 2D Ising value, and plotted $L^{1/8}\langle|O|\rangle$ vs $(\beta-\beta_c)L$ for various choices of T_c. We find the scaling behavior shown in Fig. 4(a) when $T_c = 0.4$ and from the deviations at other values of T_c estimate that $T_c = 0.4 \pm 0.1$ for $t = V = 1$. Figures 4(b) and 4(c) show similar scaled plots for $S(\pi,\pi)$ and α using $T_c = 0.4$ and the appropriate Ising indices $2-\eta = \frac{7}{4}$ and $\gamma = \frac{7}{4}$. It can be seen that these scaling parameters bring the data for our different sized lattices into reasonable agreement.

There remain a number of interesting questions regarding quantum lattice gases which can be explored using simulation techniques.[5] The band structure, and hence the nesting properties of the Fermi surface, can be changed. Naturally, the lattice structure can also be changed and different band fillings studied. We also expect interesting behavior for an attractive interaction, $V < 0$.

ACKNOWLEDGMENTS

We would like to acknowledge useful discussions with J. Cardy, J. Hirsch, and E. Loh, Jr. This work was supported in part by Department of Energy Contracts No. DE-AT03-83ER45008 and No. DE-AT03-81ER40029, National Science Foundation Grants No. PHY80-18938 and No. PHY77-27084 supplemented by funds from the National Aeronautics and Space Administration. We gratefully acknowledge E. I. Du Pont de Nemours and Company and Xerox Corporation for their support.

[1]R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D 24, 2278 (1981); D. J. Scalapino and R. L. Sugar, Phys. Rev. B 24, 4295 (1981).

[2]The 8×8 lattice corresponds to 64 sites and thus with the same amount of computing time one could also study a three-dimensional 4×4×4 lattice. Naturally one would like to go to larger systems, and with further improvements in algorithms and the coming generation of array processors this will be possible.

[3]J. Hirsch, Phys. Rev. B 28, 4059 (1983).

[4]M. E. Fisher and M. N. Barber, Phys. Rev. Lett. 28, 1516 (1972); M. N. Barber, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. L. Lebowitz (Academic, New York, 1983).

[5]J. E. Hirsch has recently reported simulations on the 2D Hubbard model using similar techniques [Phys. Rev. Lett. 51, 1900 (1983)].