Extended Hubbard model in two dimensions

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The two-dimensional half-filled extended Hubbard model is studied by means of Quantum Monte Carlo simulation. The model includes the on-site electron interaction (U) and nearest-neighbor interaction (V). We study the formation of antiferromagnetic, charge-density-wave, and superconducting states of the model as the parameters of the model are varied.

I. INTRODUCTION

The one-dimensional extended Hubbard model has been extensively studied by many people using different methods.[1-9] Among these are renormalization-group techniques,[2] Monte Carlo simulation methods,[6,7] and exact solutions for small clusters.[8,9] Despite the apparent simplicity of the extended Hubbard model, there is a rich ground-state phase diagram in terms of the interactions U and V. The ground state of the system can be a spin-density wave (SDW), charge-density wave (CDW), or superconducting state. One important feature of the phase diagram is that there is a SDW-to-CDW transition[2,6] near the line $U=2V$ for $U>0$. In this paper, we study the same extended Hubbard model in a two-dimensional square lattice by Monte Carlo simulation techniques. We find the 1D and 2D cases are qualitatively similar. However, the SDW-to-CDW transition is found near the line $U=4V$ for $U>0$ due to the change in the number of neighbors. In the following sections, we will briefly discuss the method used and present some results obtained from the simulations. We only consider the half-filled case here. The system is a 4×4 cluster with periodic boundary conditions.

II. MODEL AND METHOD

The model is defined by the Hamiltonian:

$$H=t\sum_{\substack{\langle ij\rangle\\ \mu}} C^{+}_{i,\mu}C_{j,\mu}+U\sum_{i} n_{i\uparrow}n_{i\downarrow}+V\sum_{\langle ij\rangle} n_i n_j \ , \tag{1}$$

where $\langle ij\rangle$ denotes nearest neighbors, and μ denotes spins. The first two terms together define the simple Hubbard model with an on-site electron interaction U. V measures the interaction between electrons on the neighboring sites. We chose the scale of energies so that $t=1$.

To perform Monte Carlo simulations for the model, we write the partition function of the system as:

$$\begin{aligned} Z&=\mathrm{Tr}\, e^{-\beta(H-\mu_c N)}\\ &=\mathrm{Tr}\prod_{l=1}^{L} e^{-\Delta\tau(H_0+H')}\\ &\simeq \mathrm{Tr}\prod_{l=1}^{L} e^{-\Delta\tau H_0}e^{-\Delta\tau H'} \ , \end{aligned} \tag{2}$$

where $\beta=L\Delta\tau$, μ_c is the chemical potential, and

$$H_0=t\sum_{\substack{\langle ij\rangle\\ \mu}} C^{+}_{i,\mu}C_{j,\mu} \ ,$$

$$H'=U\sum_i n_{i\uparrow}n_{i\downarrow}+V\sum_{\langle ij\rangle} n_i n_j-\mu_c\sum_i n_i \ .$$

The thermal parameter β is divided into L "imaginary time" intervals. The last step in (2) employs the Trotter approximation. The error caused by this breakup is of the order $(\Delta\tau)^2$.

The electron-electron interaction can be eliminated through the use of the discrete forms of the Hubbard-Stratonovich transformations:[10] For $U>0$

$$e^{-\Delta\tau U n_{i,\mu}n_{j,\mu'}}=\frac{1}{2}\sum_{\sigma=\pm1}\exp\left[\lambda\sigma(n_{i,\mu}-n_{j,\mu'})-\frac{\Delta\tau U}{2}(n_{i,\mu}+n_{j,\mu'})\right] \tag{3}$$

with

$$\cosh(\lambda)=\exp(\Delta\tau U/2) \ .$$

For $U<0$

$$e^{-\Delta\tau U n_{i,\mu}n_{j,\mu'}}=\frac{1}{2}\sum_{\sigma=\pm1}\exp[\lambda\sigma(n_{i,\mu}+n_{j,\mu'})-\lambda'(n_{i,\mu}+n_{j,\mu'})] \tag{4}$$

with

$$e^{-\Delta\tau U}=\cosh(2\lambda)/\cosh^2(\lambda), \quad \lambda'=\ln(\cosh\lambda) \ .$$

One auxiliary Ising variable $\sigma_0(i,l)$ is introduced at lattice site (i,l) for the interaction U, while for terms involving the interaction V,

$$Vn_i n_j=\sum_{\mu,\mu'} Vn_{i,\mu}n_{j,\mu'} \ ,$$

four auxiliary Ising variables $(\sigma_1,\sigma_2,\sigma_3,\sigma_4)$ are needed between each pair of nearest neighbors. The increased number of Ising variables in this system, as compared to the pure Hubbard model, is one of the factors limiting the size of the system we can consider. Taking the trace over fermion degrees of freedom yields:[11,12]

$$Z=\sum_{\sigma_0,\sigma_1,\sigma_2,\sigma_3,\sigma_4}\prod_{\mu=\uparrow,\downarrow}\det O_\mu[\sigma_0(i,l),\sigma_1(\langle ij\rangle,l),\sigma_2(\langle ij\rangle,l),\sigma_3(\langle ij\rangle,l),\sigma_4(\langle ij\rangle,l)] \tag{5}$$

where the O_μ are $N\times N$ matrices (N is the number of sites).

$$O_\mu=I+\prod_{l=1}^{L}(e^{-\Delta\tau K}e^{V^{l,\mu}}) ,$$
$$(K)_{i,j}=\begin{cases}1 & \text{for } \langle ij\rangle ,\\ 0 & \text{otherwise} ,\end{cases} \tag{6}$$

and $V^{l,\mu}(\sigma_0,\sigma_1,\sigma_2,\sigma_3,\sigma_4)$ corresponds to the potential due to the auxiliary Ising fields.

We use the determinant algorithm of Blankenbeler, Scalapino, and Sugar[12] to sum over the Ising spins. This algorithm involves updating the Green's function $G_\mu=0_\mu^{-1}$, when a move $\sigma\rightarrow-\sigma$ is accepted.

The Green's function G_μ satisfies the Dyson equation:

$$G'_\mu=G_\mu+(G_\mu-I)(e^{V'^\mu-V^\mu}-I)G'_\mu . \tag{7}$$

Following Hirsch's[11] procedure for the Hubbard model, we can obtain various correlation functions of interest for the present model.

The calculations are made for the half-filled case only. The total number of electrons in the system is 16. Electron-hole symmetry exists in this case, and the chemical potential $\mu_c=U/2+4V$ at all temperatures. The time slices are taken so that $\Delta\tau\max(U,4V)=0.4$. A typical Monte Carlo run for a square (4×4) cluster involved 2000–4000 measurements separated by two Monte Carlo sweeps, and proceeded by 1000 warm up sweeps. Calculations were made on the LSU FPS-264 and IBM-3084 systems.

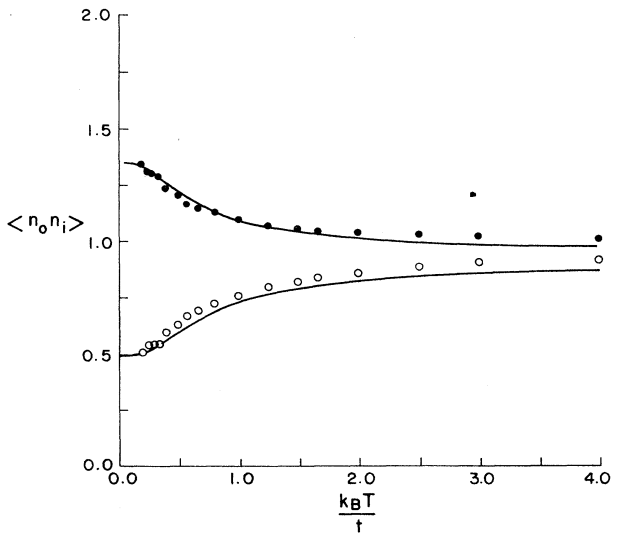

FIG. 1. First (lower curve) and second neighbor (upper curve) charge correlation functions as a function of temperature for a ring of eight sites. Solid curves are the results of an exact diagonalization calculation; closed circles and open circles are the Monte Carlo results. Parameters: $U=2$, $V=1.5$.

As a test of the program, some comparisons were made with results of exact diagonalization calculations for some small clusters. Figure 1 shows the results of one of these comparisons, in which the first and second neighbor charge correlation functions are shown for a ring of eight sites in the case $U=2.0$, $V=1.5$. The agreement is reasonably good, particularly at low temperatures. The small discrepancies (about 5%) at higher temperatures are attributed to the fact that the thermal properties in the exact diagonalization calculation are obtained using a canonical ensemble while the Monte Carlo calculation employs a grand canonical ensemble.

In the case of a four site system (one square) we find good agreement between Monte Carlo results and those obtained from exact diagonalization using a grand canonical ensemble at all temperatures. This comparison indicates that the systematic error in the Monte Carlo calculations is about 2% for the $\Delta\tau$ we used. We conclude from this that the results for the larger systems reported below have possible systematic errors of a few percent.

Statistical errors in correlation functions are estimated as about 1% at low temperatures where the correlations are large, and somewhat larger when the correlations are small at high temperatures. This error is usually smaller than the size of the dots used in our graphs. For this reason we do not supply error bars. The errors in susceptibilities can be somewhat larger as a result of numerical cancellation occurring in sums of correlation functions.

III. RESULTS

We have considered the model in different range of the parameters U and V. Various correlation functions and susceptibilities are obtained from the simulations. The quantities studied are defined as: Local moment,

$$\langle S^2\rangle=\langle(n_{i,\mu}-n_{i,-\mu})^2\rangle , \tag{8}$$

one site charge correlation,

$$\langle n^2\rangle=\langle(n_{i,\mu}+n_{i,-\mu})^2\rangle , \tag{9}$$

magnetic correlation function,

$$S(\mathbf{k})=\frac{1}{N}\sum_{ij}e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\langle(n_{i\uparrow}-n_{i\downarrow})(n_{j\uparrow}-n_{j\downarrow})\rangle , \tag{10}$$

charge correlation function,

$$S_c(\mathbf{k})=\frac{1}{N}\sum_{ij}e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\langle(n_i-\bar{n}_i)(n_j-\bar{n}_j)\rangle , \tag{11}$$

where $\bar{n}_i$ is the average number of particles on site i. Zero-frequency magnetic susceptibility,

$$\chi(\mathbf{q})=\frac{1}{N}\int_0^\beta d\tau\sum_{ij}e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\langle[n_{i\uparrow}(\tau)-n_{i\downarrow}(\tau)]\times[n_{j\uparrow}(0)-n_{j\downarrow}(0)]\rangle , \tag{12}$$

zero-frequency charge susceptibility,

$$\chi_c(\mathbf{q})=\frac{1}{N}\int_0^\beta d\tau \sum_{ij} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\langle [n_i(\tau)-\bar{n}_i][n_j(0)-\bar{n}_j]\rangle \ , \tag{13}$$

We also calculate some pairing correlation functions and susceptibilities for the system.

The singlet pairing susceptibility is

$$\chi_p(\mathbf{q})=\frac{1}{N}\int_0^\beta d\tau \sum_{ij} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)} \times\langle C_{i\uparrow}(\tau)C_{i\downarrow}(\tau)C^+_{j\downarrow}(0)C^+_{j\uparrow}(0)\rangle \ . \tag{14}$$

For $\mathbf{q}=0$,

$$\chi_p(0)=\frac{1}{N}\int_0^\beta d\tau \sum_{ij}\langle C_{i\uparrow}(\tau)C_{i\downarrow}(\tau)C^+_{j\downarrow}(0)C^+_{j\uparrow}(0)\rangle =\frac{1}{N}\int_0^\beta d\tau \sum_{\mathbf{k},\mathbf{k}'}\langle C_{\mathbf{k}\uparrow}(\tau)C_{\mathbf{k}\downarrow}(\tau)C^+_{\mathbf{k}'\downarrow}(0)C^+_{-\mathbf{k}'\uparrow}(0)\rangle \ . \tag{15}$$

We will confine our attention here to $\mathbf{q}=0$ (uniform case), and $\mathbf{q}=(\pi,\pi)$ (staggered case). We will refer to $S(\pi)$ and $\chi(\pi)$ as the staggered correlation function and the staggered susceptibility, respectively.

The staggered magnetic susceptibility will diverge at low temperature if the system is in an antiferromagnetic state, and the staggered charge susceptibility will diverge at low temperature if the system is in a charge-density-wave state. If the system is in the singlet superconducting state, the pairing susceptibility should diverge at low temperatures.

A. $U>0$, $V=0$

This is the ordinary single band Hubbard model, which has been studied in the square geometry considered here by Hirsch[11] and by Hirsch and Tang[13] for systems up to 8×8 in size. There has recently been considerable controversy concerning the ground state following the suggestion of Anderson that the ground state of the spin-$\frac{1}{2}$ two-dimensional Heisenberg antiferromagnet might lack long-range order.[14] As the systems we consider are not large, and the calculations are restricted to temperatures $k_BT/t>0.25$, we do not attempt to reach a conclusion on this point. However, our results are in agreement with those of Hirsch[11,13] showing the building up of strong antiferromagnetic correlations at low temperature, and a strongly diverging staggered magnetic susceptibility. We take the opportunity to introduce the reader to our approach to the presentation and analysis of data beginning with this rather well studied case.

Figure 2 shows the reciprocals of both the uniform and the staggered magnetic susceptibilities for $U=4$. The straight lines through the higher-temperature data points are linear least-square fits to the data points with $k_BT/t>1.5$. It is apparent that, above $k_BT/t=1.25$ for the uniform case and $k_BT/t>1.00$ for the staggered

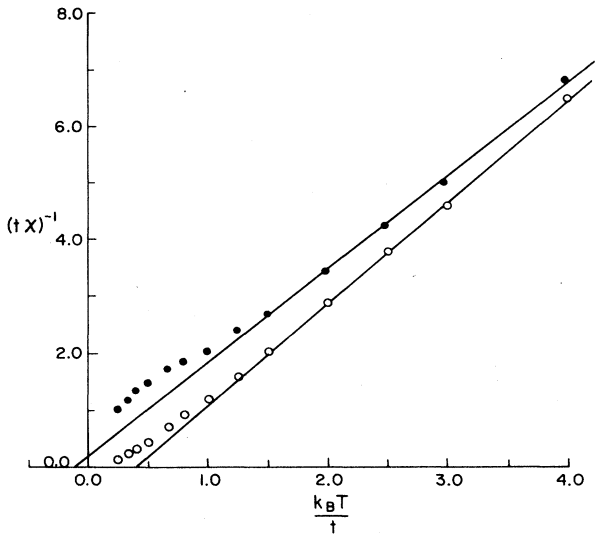

FIG. 2. Uniform (closed circles) and staggered (open circles) reciprocal magnetic susceptibility for the case $U=4$, $V=0$. The straight lines are least-squares fits to the data points for $k_BT/t\geq1.5$. The intercepts are at $k_B\Theta/t=-0.17\pm0.07$ and 0.39 ± 0.01, respectively.

case, Curie-Weiss laws apply reasonably well,

$$\chi^{-1}=[T-\Theta]/C \ . \tag{16}$$

One sees that Θ is negative (the least-squares fit value is $\Theta=-0.17\pm0.07$) for the uniform susceptibility. This is typical of antiferromagnets. On the other hand, Θ is positive (0.39 ± 0.01) for the staggered susceptibility, indicating a possible divergence and a phase transition. However, one sees a tail on the susceptibility so that χ^{-1} does not reach zero. This is, in part, a result of the finite size of the sample we consider. In addition, it has been demonstrated many years ago that the two-dimensional Heisenberg antiferromagnet with finite-range interactions can not have long-range two-sublattice order at finite temperature.[15]

The reciprocal of the uniform susceptibility, $\chi^{-1}(0)$ deviates from linear behavior in the range of temperatures where the linear fit to $\chi^{-1}(\pi)$ is approaching zero. This behavior is similar to that observed in exact[16] diagonalization calculations for the Hubbard model on small clusters. In a bulk three-dimensional antiferromagnet, $\chi^{-1}(0)$ has a sharp minimum (cusp) at the Néel temperature and approaches a finite limit as $T\to0$. Some recent results for the square lattice Heisenberg antiferromagnet[17] imply that $\chi^{-1}(0)$ should also have a minimum at finite temperatures and approach a finite limit at $T=0$. The present results are only partly consistently with these expectations, but it is plausible that the deviations are due principally to finite size effects.

B. $U=0$, $V>0$.

In this case the system appears to approach a state [usually described as a charge density wave (CDW)] in which sites are alternately almost doubly occupied or al-

most empty. The nearest neighbors of a doubly occupied site would be empty, and the second neighbors occupied, and so on, conceptually similar to a two sublattice antiferromagnet.

We show in Fig. 3(a) the development of double occupancy with decreasing temperature. Three different values of V: 0.50, 0.75, and 1.00 are considered. The tendency toward double occupancy obviously increases with increasing V and decreasing temperature. For the two larger values of V, there are indications of saturation of $\langle n^2 \rangle$ at low temperatures.

At first sight, it may appear surprising that the high-temperature limit of $\langle n^2 \rangle$ is not 1. However, a simple argument shows that the correct value is 3/2 when the electrons are uncorrelated. (In a large system in which the number of electrons equals the number of sites, if one electron is on a given site, the probability that another one will be present is only $\frac{1}{2}$ because only one spin state is available there, whereas other sites have two states). If $\langle n^2 \rangle$ is calculated for the case studied in Sec. III A, above ($U>0$, $V=0$) the high-temperature limit for $\langle n^2 \rangle$ is approached from below rather than from above.

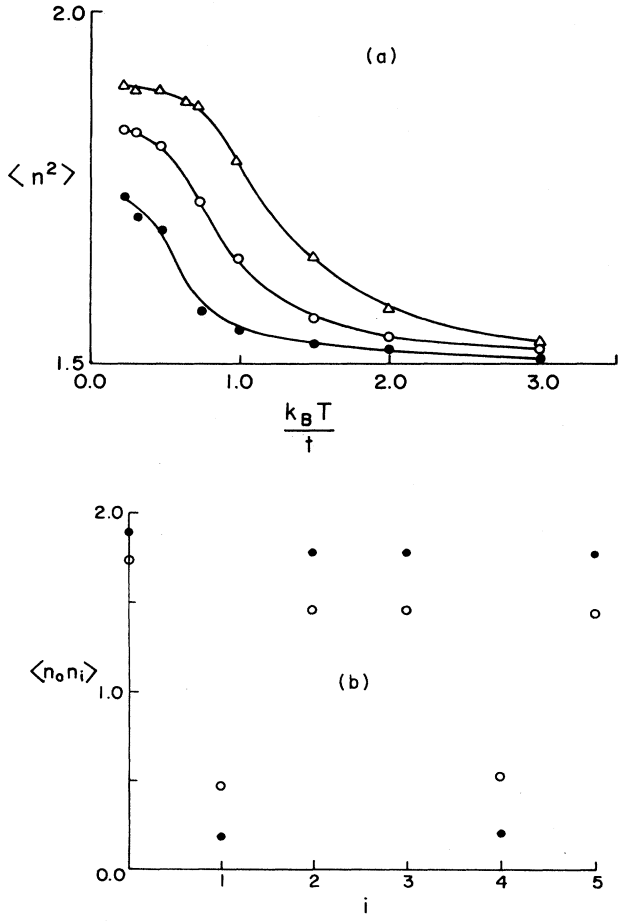

FIG. 3. (a) The development of partial double site occupancy for $U=0$, $V>0$ as the temperature decreases is illustrated by the plot of the average of the square of the site occupation number. Closed circles $V=0.5$; open circles: $V=0.75$; triangles: $V=1.0$. The curves are guides to the eye only. (b) The charge correlation function is shown for the central site and first through fifth neighbors for $U=0$, and $k_B T/t=0.25$. Open circles: $V=0.50$, closed circles, $V=1.0$.

Figure 3(b) shows the dependence of the charge correlation function for neighboring sites on distance for $V=0.5$ and 1.0 at $k_B T/t=0.25$. It is seen that if site "0" is occupied, first and fourth neighbors have depressed occupancy, and second, third, and fifth neighbors have enhanced occupancy. Increasing V increases the magnitude of the charge alternation. Perhaps, the most interesting point about Fig. 3(b) is that the magnitude of the alternation does not show any appreciable decrease with distance over the range considered.

In addition, the reciprocal staggered charge susceptibility χ_c^{-1} will approach zero, similar to the staggered magnetic susceptibility in III A above. We will show this behavior in the next subsection.

C. $U>0$, $V>0$.

The intersecting physics in this region is the competition between U and V, leading to a transition between spin-ordered and charge-ordered states. In one dimension, this crossover occurs near or on the line $U=2V$. Analytic approximations[1,2,5,9] show a transition exactly on the line $U=2V$, while Monte Carlo simulations[6] indicate small deviations from this line for intermediate values of U.

In the present case of a two-dimensional square lattice, we find a similar transition near $U=4V$. Unfortunately, we can not carry this calculation to low enough temperatures or larger systems to determine accurately the exact location and order of the transition.

Figure 4(a) shows the behavior of the quantity

$$m=\left\langle \left[N^{-1} \sum_i e^{i\mathbf{k}\cdot\mathbf{R}_i} \cdot n_i \right]^2 \right\rangle = \frac{1}{N} S_c(\mathbf{k}) , \tag{17}$$

for $\mathbf{k}=(\pi,\pi)$ as a function of V for the cases $U=2$ and $U=4$. For small V, m is small (in the range between 0.1 and 0.2), but begins a rapid rise near $U=4V$ to approach 1 for large V.

Figure 4(b) compares the behavior of staggered spin and charge susceptibilities for $U=4$ and $V=0.5$, 1.0, and 1.25 as functions of temperature. The corresponding correlation functions are shown in Fig. 4(c). For $V=0.5$, the spin susceptibility and correlation function increase rapidly at low temperatures while the charge susceptibility and correlation function remain small. When V is increased to 1.0 so that the condition $U=4V$ is satisfied both spin and charge susceptibilities and correlation functions are increasing at low temperatures, and although the spin correlations appear to be diverging more rapidly, it is not clear what will happen at $T=0$. In the case of $V=1.25$, the charge correlation function and susceptibility are strongly dominant and the spin correlation and susceptibility are being suppressed as the temperature decreases. It is evident that the system changes from spin-to-charge ordered states near $U=4V$.

At high temperatures, Curie behavior ($\chi \sim T^{-1}$) is expected for all susceptibilities in view of the expressions

for the susceptibilities, Eqs. (12)–(15) assuming that, for example,

$$\frac{1}{N}\lim_{\Delta\tau\to 0}\sum_{ij} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\langle[n_i(\tau)-\bar{n}_i][n_j(0)-\bar{n}_j]\rangle \quad (18)$$

is finite. Terms of first order in τ (18) then determine the intercept Θ (in the extrapolated plot of χ^{-1} against T), while higher terms lead to curvature in the plot. In many bulk ferromagnetic systems, plots of $\chi^{-1}(0)$ versus T are quite linear until one gets close to the Curie temperature. The Θ determined by a straight-line extrapolation is often quite close to the actual transition temperature. In an antiferromagnet, $\chi^{-1}(0)$ would be expected to show a minimum, while the staggered susceptibility, if it could be measured, should behave similarly to the uniform susceptibility in a ferromagnet. We are not aware of any demonstration that a similar situation prevails in regard to either charge-density-wave (or superconductive) systems and there is a question as to whether a sharp phase

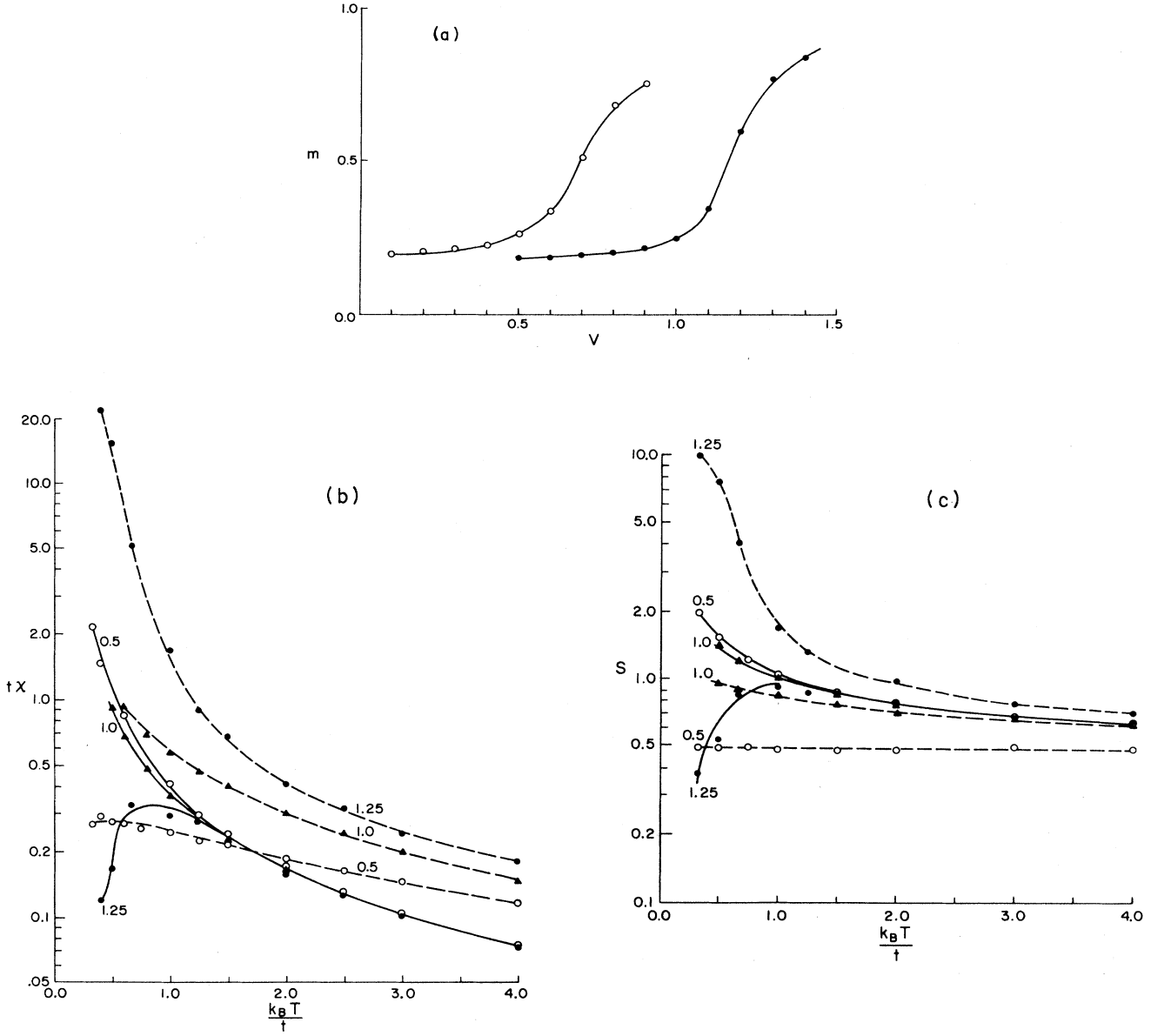

FIG. 4. (a) Behavior of the quantity m defined by Eq. (17) (essentially a staggered charge correlation function) for $U=2$ and $k_BT/t=\frac{1}{3}$ as a function of V (open circles); $U=4$ and $k_BT/t=0.5$ (closed circles). The curves are guides to the eye only. (b) Temperature dependence of staggered spin (solid lines) and charge susceptibilities (dashed lines) for $U=4$. Curves (which are guides to the eye only) are labeled by the values of V. (c) Staggered spin (solid lines) and charge (dashed lines) correlation functions as functions of temperature for $U=4$. Curves, which are guides to the eye only, are labeled by the values of V.

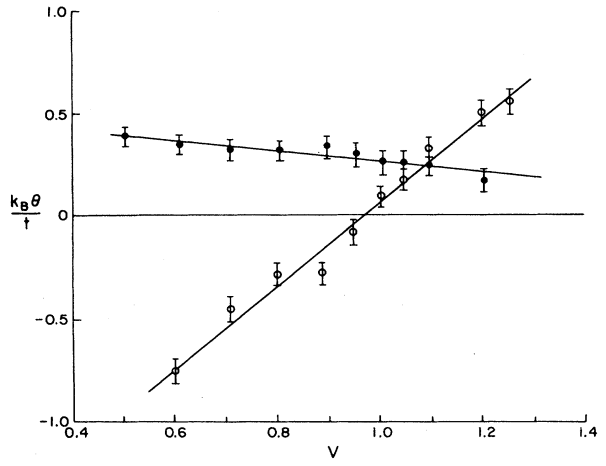

FIG. 5. Intercept Θ in a Curie-Weiss law least-squares fit to the staggered spin (closed circles) and charge susceptibilities (open circles) for $U=4$ as functions of V. Lines are guides to the eye only.

transition at a finite temperature is to be expected in any of these 2D systems. However, we think it remains informative to consider the behavior of Θ as a function of the parameters of the system.

We show in Fig. 5 the intercept Θ from the least squares fits to the staggered spin and charge susceptibilities for $U=4$ as a function of V. Clearly, for small values of V, the only indication of a susceptibility divergence at finite temperature, i.e., $\Theta>0$, occurs in the spin susceptibility. In the neighborhood of $V=1$, Θ_c becomes positive, and rapidly rises to become larger than Θ_s. We observe that Θ_s does not go to zero as V approaches 1 from below. This leads to the plausible conjecture that the transition between antiferromagnetic and charge-density-wave states is sharp as V increases.

D. $U<0$

Since the parameter U was introduced to describe electron repulsion on a single site, it seems, at first, unlikely that negative U values could arise. However, the possibility of negative U was suggested by Anderson[18] in regard to localized electronic states in amorphous semiconductors. It is also possible that effective negative U's could arise as a result of competing electronic interactions, for example, including polarization effects.[19] Mathematically, the negative U case has attracted some interest in that superconductivity is expected to result.[20] We have considered negative U's in these calculations.

We shall see below that the boundary between dominance of charge and pairing correlations is either exactly at or at least very close to $V=0$, and that pairing remains strong for small negative values of V. (Effective negative values of V might also result from polarization effects).

In Fig. 6(a) we show the reciprocal of the staggered charge susceptibility χ_c as a function of T at $U=-4$ for some positive values of V (0.2, 0.5, and 1.0). These susceptibilities suggest the possibility of a divergence at low temperatures. The value of the intercept of a linear least squares fit increases with V, although all cases show substantial deviations from linear behavior for low temperatures or small χ_c^{-1}. Figure 6(b) shows the development of

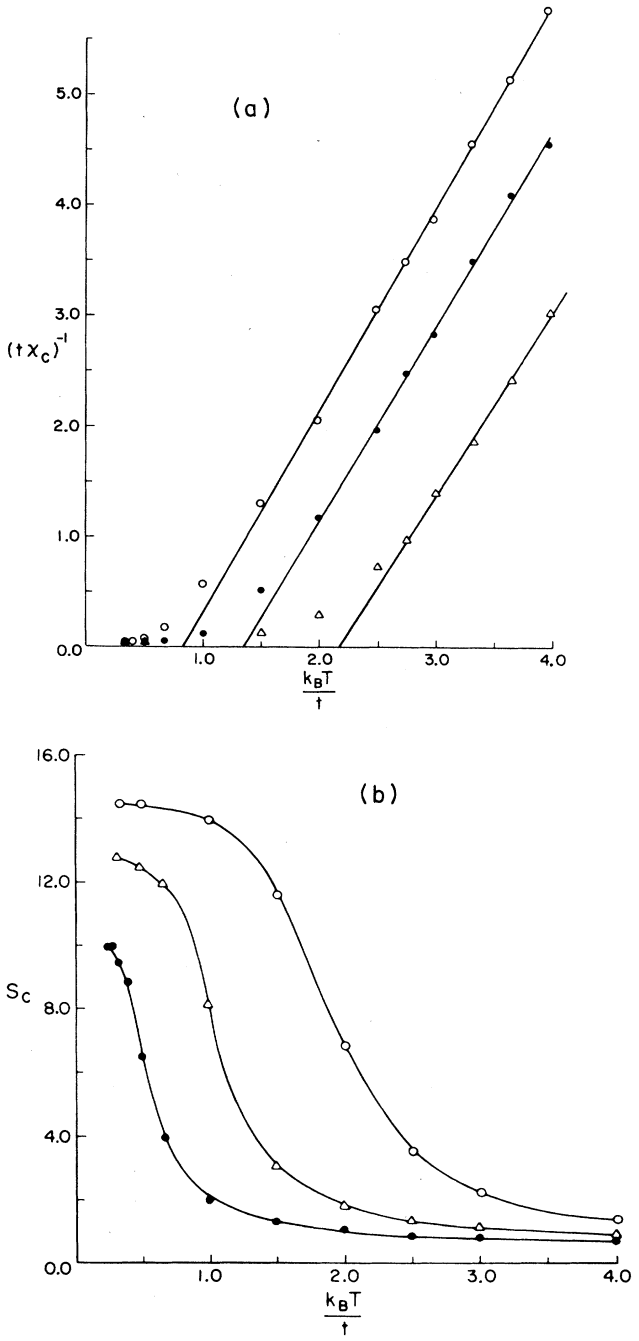

FIG. 6. (a) Reciprocal of the staggered charge susceptibility for $U=-4$ and $V=0.2$ (open circle), 0.5 (closed circles), and 1.0 (triangles). Lines are least-squares fits to the data points at high temperatures. (b) Staggered charge correlation functions as functions of temperature for $U=-4$. $V=0.2$ (closed circles), 0.5 (triangles), and 1.0 (open circles). Curves are guides to the eye only.

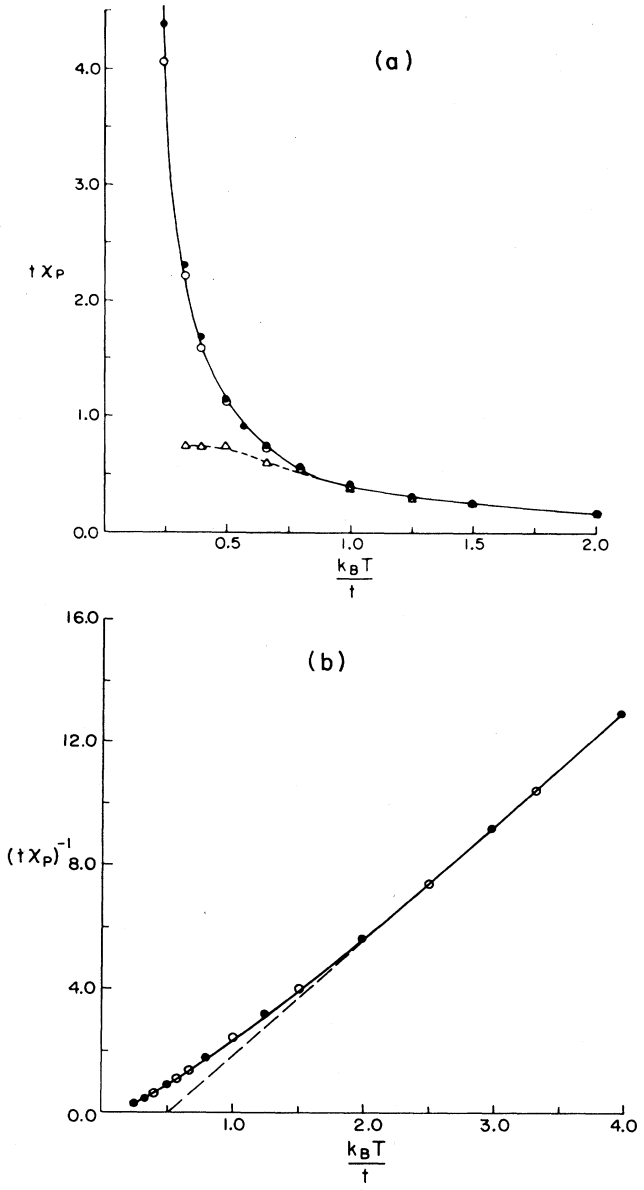

FIG. 7. (a) Singlet pairing susceptibility as functions of temperature for $U=-4$ and $V=0.2$ (triangles) 0.0 (open circles), and 0.2 (closed circles). Curves are guides to the eye only. (b) Reciprocal of the singlet pairing susceptibility as a function of temperature for $U=-4$ and $V=0$ (open circles), and -0.2 (closed circles). The curve is a guide to the eye only. The straight line indicates linear extrapolation of the high-temperature data.

the staggered charge correlation function at low temperatures in this case, indicating, we believe, the formation of a CDW state at low temperatures, as in the case of positive U when $V > U/4$. In fact, the charge correlation seems to be enhanced by negative U. In the case of $V=1.0$, the value of S_c saturates around 14.7, close to the maximum possible value of 16.

When $V=0$, there is a direct mapping from the antiferromagnetic state for $U>0$ to the CDW state for $U<0$, in which the S_z-S_z correlations in the antiferromagnetic case transform into charge correlations in the CDW state.[11] At the same time, long-range singlet pairing correlations of the superconducting type develop so that it is apparently possible to have both charge order and superconducting order in the ground state. This appears explicitly in exact diagonalization calculations for small systems.[21]

Figure 7(a) shows the pairing susceptibility $\chi_p(0)$, (Eq. 14) as a function of temperature for $U=-4$ and $V=0.2$, 0.0, and -0.2. It is seen that the pairing correlations are suppressed for small positive V, but are possibly slightly enhanced by a small negative V. Figure 7(b) shows the reciprocal of the pairing susceptibility for $U=-4$ and $V=0.0$ and -0.2. The results are very close. As in the case of the other susceptibility it appears that a kind of Curie-Weiss law is reasonably well satisfied at high temperatures ($k_BT/t>2.0$).

It would be interesting to explore the entire phase diagram of the extended Hubbard model, including the region of large negative V. In the present Monte Carlo simulation the algorithm appears to become unstable for negative V as the magnitude of V becomes larger. This may be an indication of an approach to a condensed phase, but we are unable to proceed further.

IV. CONCLUSIONS

We have performed Monte Carlo simulation calculations for the extended Hubbard model on a square lattice. Only the half-filled case is considered here. We have studied properties of the model in different regions of its phase diagram, and observed the formation of AF, CDW, and singlet pairing states. An AF-to-CDW transition is found near the line $U=4V$ for positive U. Singlet pairing of the superconducting type becomes significant for negative U and $V\leq 0$, but disappears when $V>0$. The overall picture in two dimensions is similar to that in one dimension.

ACKNOWLEDGMENTS

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[1]J. Solyom, Adv. Phys. **21**, 201 (1979).
[2]V. J. Emery, in *Highly Conducting One-Dimensional Solids*, edited by J. Devreese, R. Evrard, and V. van Doren (Plenum, New York, 1979).
[3]P. Pincus, P. Chaikin, and C. Coll, Solid State Commun. **12**, 1265 (1973).
[4]V. J. Emery, Phys. Rev. B **14**, 2989 (1976).
[5]R. A. Bari, Phys. Rev. B **3**, 2662 (1971).

[6]J. E. Hirsch, Phys. Rev. Lett. **53**, 2327 (1984).
[7]H. Q. Lin and J. E. Hirsch, Phys. Rev. B **33**, 8155 (1986).
[8]B. Fourcade and G. Spronken, Phys. Rev. B **29**, 5096 (1984).
[9]L. M. del Bosch and L. M. Falicov, Phys. Rev. B **37**, 6073 (1988).
[10]J. E. Hirsch, Phys. Rev. B **28**, 4059 (1983).
[11]J. E. Hirsch, Phys. Rev. B **31**, 4403 (1985).
[12]R. Blankenbeler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D **24**, 2278 (1981).
[13]J. E. Hirsch and S. Tang, Phys. Rev. Lett. **62**, 591 (1989).
[14]See, for example, S. Liang, B. Doucot, and P. W. Anderson, Phys. Rev. Lett. **61**, 365 (1988).
[15]N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966).
[16]J. Callaway, Physica **149B**, 17 (1988).
[17]A. Auerbach and D. P. Arovas, Phys. Rev. Lett. **61**, 617 (1988).
[18]P. W. Anderson, Phys. Rev. Lett. **34**, 953 (1975).
[19]J. Callaway, D. G. Kanhere, and P. K. Misra, Phys. Rev. B **36**, 7141 (1987).
[20]P. Noziéres and S. Schmitt-Rink, J. Low. Temp. Phys. **59**, 195 (1985).
[21]J. Callaway, D. P. Chen, and D. G. Kanhere (unpublished).