# Two-Dimensional Negative-$U$ Hubbard Model

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Quantum Monte Carlo simulations are used to explore the phase diagram of the negative-$U$ Hubbard model. As the system is doped away from half filling, $\langle n\rangle=1$, the $s$-wave pair-field correlations are enhanced and the charge-density-wave correlations suppressed. There is no indication of phase separation. Away from half filling, the pair-field correlations are consistent with Kosterlitz-Thouless scaling and a finite $T_c$ which peaks near $\langle n\rangle=1$ but vanishes at exactly half filling.

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The phase diagram of the two-dimensional negative-$U$ Hubbard model depends upon $|U|/t$ and the band filling $n=\langle n_{i\uparrow}+n_{i\downarrow}\rangle$. It is believed to consist of a zero-temperature superconducting–charge-density-wave (CDW) "supersolid" line for half filling $\langle n\rangle=1$ and a finite-temperature Kosterlitz-Thouless superconducting phase at all other fillings, with $T_c$ going to zero as $\langle n\rangle$ goes to 0 or 2. The phase diagram is symmetric about half filling $\langle n\rangle=1$ because of particle-hole symmetry. This picture has had some limited numerical support. It has been previously shown that at half filling[1,2] the $\mathbf{q}=(\pi,\pi)$ charge-density-wave and the $s$-wave pair-field correlations have long-range order in the ground state. In addition,[2] the quarter-filled $\langle n\rangle=0.5$ band was found to have long-range $s$-wave pair-field order in the ground state. Here we present further results obtained from Monte Carlo simulations which provide additional insight into this interesting many-body problem.

The Hamiltonian of the negative-$U$ Hubbard model on a two-dimensional square lattice with a nearest-neighbor one-electron overlap matrix element $t$ is

$$H=-t\sum_{\langle i,j\rangle,s}(c_{is}^{\dagger}c_{js}+c_{js}^{\dagger}c_{is})-|U|\sum_i(n_{i\uparrow}-\tfrac{1}{2})(n_{i\downarrow}-\tfrac{1}{2})-\mu\sum_{i,s}n_{is}\,. \qquad (1)$$

Here $c_{is}$ destroys an electron of spin $s$ on site $i$, $|U|$ is the strength of the attractive on-site interaction, and $\mu$ is the chemical potential which determines the band filling $n$. With our convention for the interaction, the half-filled band has $\mu=0$.

There are two important types of correlations, charge-density and $s$-wave pairing. To characterize these we have studied the equal-time charge-density structure factor

$$C(\mathbf{q})=\langle\rho_{\mathbf{q}}\rho_{\mathbf{q}}^{\dagger}\rangle\,, \qquad (2)$$

with

$$\rho_{\mathbf{q}}^{\dagger}=\frac{1}{\sqrt{N}}\sum_l e^{i\mathbf{q}\cdot l}(\langle n_{l\uparrow}+n_{l\downarrow}\rangle) \qquad (3)$$

and the $\mathbf{q}=0$ equal-time $s$-wave pair-field correlation function

$$P_s=\langle\Delta^{\dagger}\Delta+\Delta\Delta^{\dagger}\rangle\,, \qquad (4)$$

with

$$\Delta^{\dagger}=\frac{1}{\sqrt{N}}\sum_l c_{l\uparrow}^{\dagger}c_{l\downarrow}^{\dagger}\,. \qquad (5)$$

The variation of the pairing and charge-density-wave

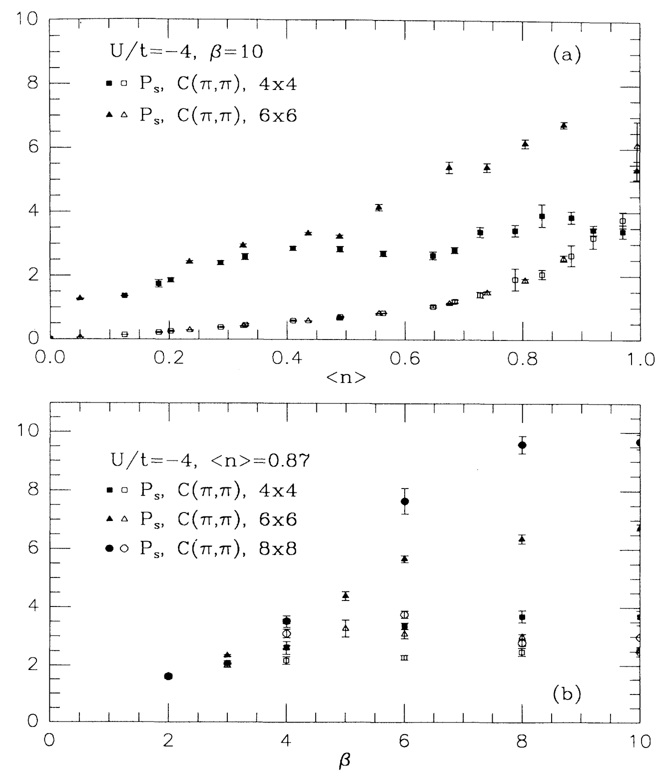


FIG. 1. (a) Pairing ($P_s$) and charge-density-wave [$C(\pi,\pi)$] correlations as a function of the filling $\langle n\rangle$ for 4×4 and 6×6 lattices with $U=-4$, $t=1$, and $\beta=10$. (b) Pairing ($P_s$) and charge-density-wave [$C(\pi,\pi)$] correlations as a function of the inverse temperature $\beta$ at a filling $\langle n\rangle=0.87$ for $U=-4$ and $t=1$ on 4×4, 6×6, and 8×8 lattices.

correlations with the electron site density $\langle n \rangle$ is illustrated in Fig. 1(a). Here $P_s$ and $C(\pi,\pi)$ are shown versus $\langle n \rangle$ for $U/t=-4$ and $\beta=10$ for 4×4 and 6×6 lattices. At $\langle n \rangle=1$, we have $P_s=C(\pi,\pi)$ within error bars as expected for the half-filled band. As previously discussed, a finite-size scaling analysis of $P_s$ and $C(\pi,\pi)$ for $\langle n \rangle=1$ has shown that the system has long-range pairing and charge-density-wave order in the ground state.[1,2] As $\langle n \rangle$ decreases from 1, the charge-density-wave correlations at $\mathbf{q}=(\pi,\pi)$ are suppressed, while the pairing correlations are initially enhanced. Figure 1(b) shows the temperature dependence of $P_s$ and $C(\pi,\pi)$, with $\langle n \rangle=0.87$ for 4×4, 6×6, and 8×8 lattices with $|U|/t=4$. Here we see that $P_s$ increases at low temperatures, saturating at a value which increases with the size of the lattice. The charge-density structure factor $C(\pi,\pi)$, on the other hand, settles down to a low-temperature value which is essentially independent of the lattice size, implying that the charge-density correlations are short range. It even appears that $C(\pi,\pi)$ decreases slightly at large values of $\beta$, where the long-range pair-field correlations develop. This could reflect the opening of a superconducting gap in the single-particle spectrum.

As discussed, we expect that the negative-$U$ Hubbard model away from half filling will undergo a finite-temperature Kosterlitz-Thouless[3] transition into a superconducting phase. In this case, $P_s$ would scale as

$$P_s = N_x^{2-\eta} f(N_x/\xi)\,, \tag{6}$$

with $N_x$ the linear lattice dimension, $\eta=0.25$, and $\xi \sim \exp[A/(T-T_c)^{1/2}]$. In Figs. 2(a) and 2(b), we show $P_s$ data with $U/t=-4$ for $\langle n \rangle=0.87$ and $\langle n \rangle=0.5$ scaled according to Eq. (6). In both cases $T_c$ and $A$ were used as parameters, giving $T_c \cong 0.1$, $A=0.5$ for $\langle n \rangle=0.87$ and $T_c=0.045$, $A=0.4$ for $\langle n \rangle=0.5$. With the limitations on lattice size imposed by our present quantum Monte Carlo algorithms, these values of $T_c$ are clearly approximate. They are shown as the squared points in Fig. 3, where the superconducting Kosterlitz-Thouless temperature is plotted versus $\langle n \rangle$ for $U/t=-4$.

Near half filling we have used the analogy with a two-dimensional Heisenberg antiferromagnetic in a magnetic field to argue that

$$T_c \simeq -2\pi J/\ln|1-\langle n \rangle|\,. \tag{7}$$

In order to set the coefficient $2\pi J$, we note that in the absence of a field, the magnetic correlation length[4] (the pair-field or CDW correlation length for the negative-$U$ Hubbard model with $\langle n \rangle=1$) scales as $\exp(2\pi J/T)$, with $J$ an effective exchange parameter. Using our $\langle n \rangle=1$ results, we find that $2\pi J \simeq 0.25$. This reduction is due to both spin and charge fluctuations, as noted in Ref. 1. The dashed line in Fig. 3 corresponds to $T_c \simeq -0.25/\ln|1-\langle n \rangle|$. From Fig. 3 we estimate that the maximum $T_c$ for $|U|/t=4$ is of order $0.1t$. Based on further simulations at larger values of $|U|$, we estimate that the maximum $T_c$ for the negative-$U$ Hubbard model is of order $0.2t$ for $|U|/t \simeq 8$ and $\langle n \rangle \simeq 0.85$. For larger values of $|U|/t$, the peak value of $T_c$ falls as $t^2/|U|$.

In Fig. 4(a), $C(q_x,q_y)$ is shown versus $(q_x,q_y)$ along the path indicated in the figure for various values of $\langle n \rangle$. As $\langle n \rangle$ decreases, the peak remains at $(\pi,\pi)$, but its am-

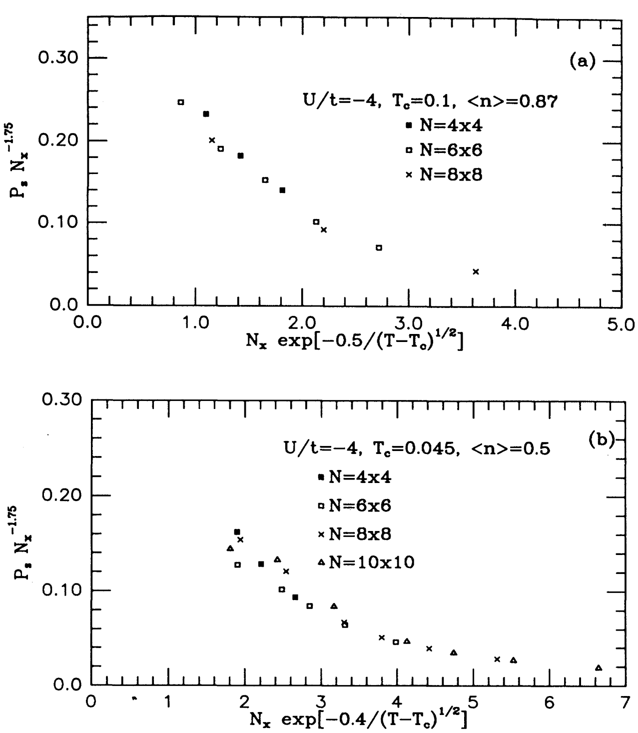


FIG. 2. (a) Pairing correlations ($P_s$) scaled according to Eq. (6) for $U=-4$, $t=1$, and $\langle n \rangle=0.87$. (b) Same as (a) with $\langle n \rangle=0.50$.

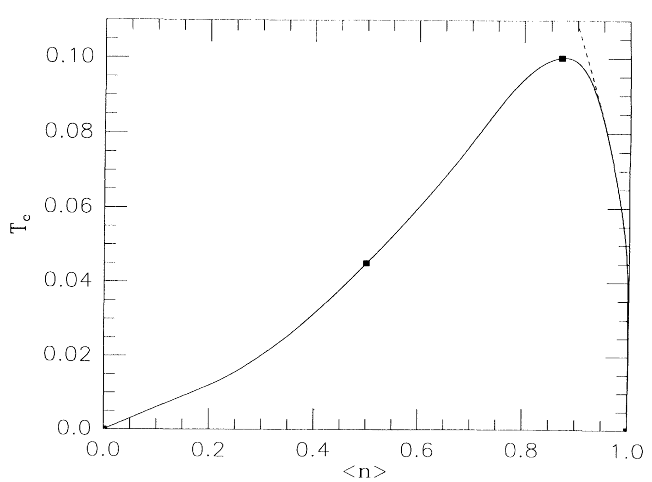


FIG. 3. $T_c$ vs $\langle n \rangle$ for $U=-4$ and $t=1$. The solid line is to guide the eye. The dashed line is $T_c=-0.25/\ln|1-\langle n \rangle|$.

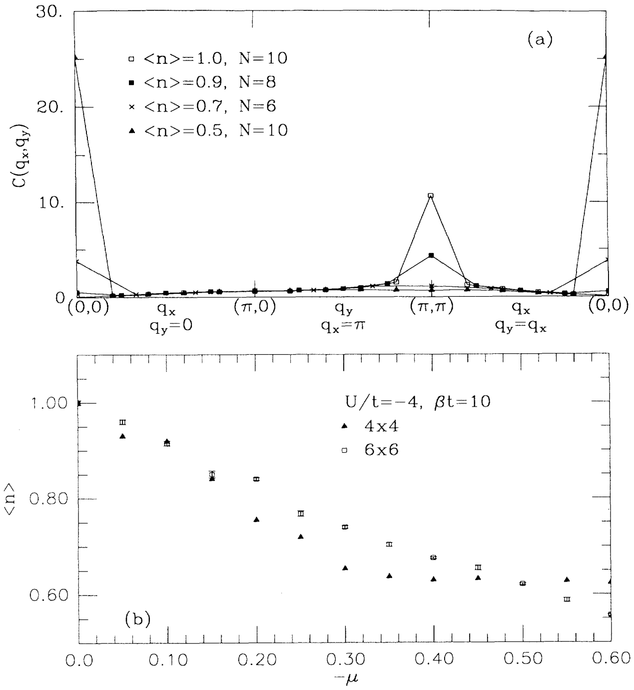


FIG. 4. (a) Charge-density-wave correlation $C(q_x,q_y)$ as a function of $(q_x,q_y)$ for different values of $\langle n\rangle$. (b) $\langle n\rangle$ vs $\mu$ for $U=-4$, $\beta=10$, and $t=1$ on $4\times4$ and $6\times6$ lattices.

plitude decreases, as previously shown in Fig. 1(a). At the same time, a peak at $\mathbf{q}=(0,0)$ begins to grow. This can be understood by remembering that a negative-$U$ Hubbard model which is doped away from half filling can be mapped onto the half-filled positive-$U$ Hubbard model in an external $z$-directed magnetic field which is proportional to $\mu$. Under this spin-down particle-hole canonical transformation $[c_{l\downarrow}\rightarrow d_{l\downarrow}^{\dagger}(-1)^l]$, $C(\mathbf{q})$ goes over to $\langle M_q^z M_q^z\rangle$ and $P_s$ goes over to $\langle M_q^x M_q^x + M_q^y M_q^y\rangle$, with $\mathbf{q}=(\pi,\pi)$. Now a half-filled positive-$U$ Hubbard model has long-range antiferromagnetic order in its ground state. In the presence of a $z$-directed magnetic field, it will undergo a spin-flop transition giving rise to a $\mathbf{q}=(0,0)$ component of the magnetization in the $z$ direction, which corresponds to the $\mathbf{q}=(0,0)$ peak in $C(q)$. The antiferromagnetic $\langle M_q^x M_q^x + M_q^y M_q^y\rangle$ correlations at $\mathbf{q}=(\pi,\pi)$ correspond to the $P_s(\mathbf{q}=0)$ pair-field correlations.

Last, we turn to the question of phase separation. In a continuum model with finite-range forces, phase separation into low- and high-density phases can occur in more than two dimensions.[5,6] However, on a lattice with only an on-site attraction, the interaction is saturated when a local pair is formed. In order to examine this in more detail,[7] we have plotted $\langle n\rangle$ vs $\mu$ for $U/t=-4$ and $\beta=10$ in Fig. 4(b). The smooth variation of $\langle n\rangle$ as $\mu$ changes suggests that there is no phase separation. In addition, a histogram of the individual Monte Carlo measurements of $n$ exhibits a single-peak instead of the two-peak behavior which would be present if there were a first-order transition. Thus we find no evidence for phase separation. It will be interesting to study an extended negative Hubbard model in which a near-neighbor attractive interaction is included. In this case, a condensed liquid phase can form, and it will be interesting to explore the competition between this phase and the superconducting phase.

Our conclusions from this study of the two-dimensional negative-$U$ Hubbard model are the following: (1) Away from half filling, $s$-wave pairing correlations are dominant, and only short-range charge-density-wave correlations occur; (2) the scaling of the pair-field correlations are consistent with a finite-temperature Kosterlitz-Thouless transition which varies with density, as indicated in Fig. 3, with a maximum $T_c$ of order $0.2t$ for $|U|/t\simeq 8$ and $\langle n\rangle\simeq 0.85$; (3) there is no indication of a phase separation as the system is doped away from half filling.

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