Spin gap and superconductivity in the three-dimensional attractive Hubbard model

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(May 26, 1994)

We study the phase diagram for the attractive (i.e., negative-U) Hubbard model on a simple cubic lattice, through Monte Carlo simulations. We obtain the critical temperature, $T_c$, for superconductivity from a finite-size scaling analysis of the data for the pairing correlations. For fixed on-site attraction, $U$, $T_c$ displays a maximum near the filling factor 0.9, roughly independent of $U$. For fixed filling we estimate the crossover temperature $T^*(U)$, separating the normal states: metallic and spin-gap. There is also a critical value $U_p$ for pair formation, the magnitude of which seems to be independent of doping. The relevance of these results to the high-$T_c$ oxides is discussed.

PACS: 71.27.+a, 74.25.Dw, 74.20.Mn, 75.10.Jm, 75.10.Lp

Phys. Rev. B 50, 1 July 1994

1.\textsuperscript{a}The Hubbard Hamiltonian can be written as

$$H = -t \sum_{\langle i,j \rangle} \left( c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.} \right) + U \sum_i \left( n_{i\uparrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right) - \mu \sum_{i,\sigma} n_{i\sigma},$$

(1)

where the sums run over sites of a simple-cubic lattice, $(i,j)$ denotes nearest neighbor sites, H.c. stands for Hermitian conjugate, and $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (annihilates) a fermion at site $i$ with spin $\sigma$; $U < 0$ is the attractive on-site interaction and $\mu$ is the chemical potential controlling the band-filling. Since the simple-cubic lattice is bipartite, the band is half-filled when the Hamiltonian (1) displays particle-hole symmetry, or $\mu = 0$. In this case, superconducting correlations in the attractive model are equivalent to planar magnetic correlations in the repulsive model\textsuperscript{6}. The strong-coupling limit of (1) can be obtained through perturbation theory in the space of doubly occupied states and is equivalent\textsuperscript{10,11} to a Heisenberg model in a transverse field proportional to $\mu$.

Here we use a grand-canonical Quantum Monte Carlo simulation; see Refs. 12–15 for details. The imaginary time is discretized through the introduction of $M$ “time” slices separated by an interval $\Delta \tau$ such that $\beta \equiv \Delta \tau M$. One should stress that the simulation for the attractive Hubbard model is free from “minus sign” problems\textsuperscript{11,14,15}. We calculate quantities such as the equal-time $\mathbf{q} = 0$ local (or s-wave) pairing correlation function,

$$P_s(T, L) \equiv \langle \Delta^\dagger \Delta + \Delta \Delta^\dagger \rangle,$$

(2)

where $T$ is the temperature, $L$ is the linear lattice size, and

$$\Delta^\dagger \equiv \frac{1}{\sqrt{N_s}} \sum_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger,$$

(3)

and the uniform magnetic susceptibility
\[ \chi_s = \frac{1}{N_s} \sum_{ij} \int_0^\beta d\tau \langle m_i(\tau)m_j(0) \rangle, \]

with

\[ m_i(\tau) = e^{-\beta H}[n_{i\uparrow} - n_{i\downarrow}]e^{-\tau H}. \]

The dependence of the pairing correlation function with the system size can be extracted through finite-size scaling (FSS) arguments. For an infinite three-dimensional system one expects a superconducting transition within the XY-model universality class, with pairing correlations decaying algebraically at the critical temperature \( T_c \). For a finite system of size \( L \), one can assume the following FSS ansatz for its associated uniform Fourier transform

\[ P_s(T, L) = L^{2-\eta} \hat{F}(L/\xi), \]

where \( \xi \) is the correlation length for the infinite system, and \( F(z) \) is a scaling function such that \( F(z) \to \text{const} \) when \( L \ll \xi \); in three dimensions, \( \eta \approx 0 \). At \( T_\text{c} \), \( \xi = \infty \), so that \( L^{-2} P_s(T_c, L) \) is a constant independent of lattice size. By plotting \( L^{-2} P_s(T, L) \) as a function of \( T \) for systems of different sizes, an estimate of \( T_c \) can be obtained as the temperature where two successive curves intercept.

Since we are interested in several values of both \( U \) and \( \rho \), we had to restrict ourselves to small systems due to our limited computer capabilities. From now on, energies will be expressed in units where the hopping \( t = 1 \), and we also set the Boltzmann constant \( k_B = 1 \).

We considered lattices with \( 4 \times 4 \times 2 \) and \( 4 \times 4 \times 4 \) sites; but in order to assess possible finite-size effects we have also performed a few runs on a \( 6 \times 6 \times 6 \) lattice. For the \( L_x \times L_y \times L_z \) lattices, one may think of several definitions for a mean linear size \( L \), such as

\[ L_1 \equiv \sqrt{3/(L_x^2 + L_y^2 + L_z^2)} \approx 2.83, \quad L_2 \equiv 3/(L_x^{-1} + L_y^{-1} + L_z^{-1}) = 3, \quad \text{and} \quad L_3 \equiv (L_xL_yL_z)^{1/3} \approx 3.17. \]

Figure 1 shows the size-scaled pairing correlation, Eq. (2), as a function of the inverse temperature, for \( U = -6 \) at half-filling and for three different lattice sizes; the data for the \( 4 \times 4 \times 2 \) lattice are plotted assuming \( L = L_2 = 3 \). One can define the inverse transition temperature, \( \beta_\text{c} \), as the value where data points for two different-sized systems (\( L, L' \)) superimpose. This implies \( T_\text{c} \approx 0.25 \) and \( T_\text{c} \approx 0.23 \) for (4,3) and (6,4) scalings, respectively; using \( L = L_3 = 3.17 \) for the smaller lattice, one would get \( T_\text{c} \approx 0.3 \) from the (4,3) scaling. The definition \( L = 3 \) for the smaller system then provides estimates for \( T_\text{c} \) that are closer to the more reliable scaling (6,4) than \( L_1 \) or \( L_3 \). Ideally a definite trend would only be detectable through the use of systems larger than \( L = 6 \), which would become prohibitively expensive in terms of computer time.

The clusters used here have \( N_s = L_x \times L_y \times L_z \) sites, with periodic boundary conditions; that is, each site is connected with its six nearest neighbors through a hopping term. The simulations were performed on Sun and IBM RISC-6000/525 workstations; a single datum point involves between 500 and 4000 MC sweeps over all time slices and we took \( \Delta \tau = 0.125 \). In a grand-canonical simulation, for each temperature the chemical potential is adjusted to obtain the desired occupation, \( \rho \equiv \langle n \rangle \).
sent the critical temperatures obtained from a \(\{4,6\}\) scaling, both with \(L = L_2\) (squares) and with \(L = L_3\) (circles). One should have in mind that at half-filling the ordered phase below \(T_c(U)\) corresponds to both superconductivity and charge ordering, since the order parameter displays full three-dimensional rotational symmetry\(^6\).

Also, the attractive model at half-filling is equivalent to the repulsive model, with the superconducting and charge order parameters becoming the planar (XY) and axial (Z) staggered magnetizations, respectively. In view of this, in Fig. 2 we compare results for \(T_c\) from the attractive model with the Néel temperature \(T_N\) for the repulsive model obtained from very extensive simulations\(^3\) (within a different extrapolation to estimate \(T_N\); open triangles), and from a Gutzwiller-type variational calculation\(^20\) (the solid line is the “bare” result \((T_N(U))\), and the dashed line is an adjustment \((3.83/6.0) \times T_N\) to fit the mean-field result to that of high-temperature series expansions for the Heisenberg model, according to which\(^4\) \(T_N \simeq 3.83t^2/|U|\)). The estimates for \(T_c\) using \(L_1\) lie below the “normalized” \(T_N(U)\) which is probably a lower bound; from now on all quoted estimates for \(T_c\) will be based on \(L_2\). For weak couplings (i.e., \(|U| < < t\), the system is in a BCS-like regime; the difference with respect to the standard BCS theory being due to the fact that quasi-particles with any wavevector can pair, not only those close to the Fermi level. Accordingly, the critical temperature is still exponentially small\(^6\), but with a different energy scale: \(T_c \sim W \exp(-W/|U|)\), where \(W = 3t\) is one half of the bandwidth.

In Fig. 3 we present the uniform susceptibility as a function of temperature for the \(L = 4\) lattice at half-filling, and for several values of \(U\). The solid line is the non-interacting result, \(\chi_s^{(0)}\), for the same lattice size; its divergence as \(T \to 0\) is due to the finite-size of the system, since \(\chi_s^{(0)}\) approaches the Pauli behavior if the \(L \to \infty\) limit is taken before \(T \to 0\). For \(U = -0.5\) and \(U = -1\), the behavior of \(\chi_s\) is similar to that of the non-interacting (metallic) case. In contrast, for \(U \leq -2\), the uniform susceptibility is suppressed below some temperature \(T^\times(U)\). This can be understood in the strong-coupling regime by noticing that local pairs are being formed and that spin excitations necessarily imply pair breaking with an energy cost \((\text{gap})\) of order \(|U|\). The formation of local pairs, and the associated spin gap, should be reflected in the magnetic properties: bound singlet pairs must have smaller response to a uniform field than isolated fermions. At intermediate couplings, this behavior can be explained along similar lines, in terms of pairing correlations\(^4\). Therefore, \(T^\times(U)\) represents a crossover temperature separating two normal-state regions: metallic and spin-gap. In Ref. 4, this crossover temperature was defined as the one at which \(\chi_s\) deviates from a renormalized Random Phase Approximation. Here we choose a different definition, which follows closely the experimental criterion based on NMR relaxation measurements, namely the temperature at which \(\chi_s\) is maximum; see e.g., the discussion in Ref. 5. The crossover line obtained this way is displayed in Fig. 2. We have compared the data in Fig. 3 with some obtained for the \(L = 6\) lattice, and found no significant finite-size effects. Nevertheless, in view of the arbitrariness of this definition, the crossover line obtained is only a crude estimate, and should be taken with care.

![FIG. 3. Uniform susceptibility as a function of temperature at half filling for a simple-cubic lattice with \(L = 4\). The symbols refer to the values of \(U\) shown, and error bars are smaller than the data points.](image)

![FIG. 4. Critical temperature as a function of the on-site coupling \(-U/t\), for \(\rho = 0.8\) (solid squares); the solid line is a guide to the eye. The dotted line is the crossover temperature \(T^\times\) (see text).](image)

As the occupation is varied, the behavior does not change drastically. For instance, in Fig. 4 we show both \(T^\times\) and \(T_c\) as functions of \(-U\), for an occupation \(\rho = 0.8\). Away from half-filling the order parameter is two-dimensional, corresponding to superconductivity alone; i.e., charge ordering is lost. While \(T^\times\) is roughly the same (within the range of \(U\) examined here) as for \(\rho = 1\), \(T_c\) is slightly higher than for the half-filled case.

A plot of \(\rho(\mu)\) for the non-interacting \(L = 4\) system at zero temperature displays several plateaux; in particular...
there is one at $\rho = 0.6875$, corresponding to 44 fermions in the system. These plateaux are still present in the interacting case, and are rounded at finite temperatures. This is a finite-size effect that should disappear in the thermodynamic limit, but nonetheless affect the data for $\rho = 0.7$ in these small systems: the uniform susceptibility is strongly suppressed for any $U < 0$. The data for $\rho = 0.6$ are free from these effects.

In conclusion, we have obtained the phase diagram in the temperature–coupling constant–occupation space for the attractive (i.e., negative-$U$) Hubbard model on a simple cubic lattice. For fixed $U$, the critical temperature for superconductivity displays a maximum at the occupation $\rho \simeq 0.9$. For fixed occupation there are two regimes: weak coupling ($|U| \ll t$), where superconductivity sets in at very low temperatures, from a normal metallic state; and intermediate- to strong-couplings, where superconductivity sets in from a spin-gap phase at higher temperatures. The changeover from a normal metal to a spin-gap phase occurs at a crossover temperature, which does not seem to be very sensitive to the occupation in the range $[0.6, 1.0]$, at least for $U \leq -4$. We have also established that the critical value of $|U|$ for pair formation lies in the interval $[-2, -1]$, for all fillings examined. With respect to the cuprates, the existence and origin of the superconducting gap has not been fully settled yet. If the spin gap, which opens above (and not at) $T_c$ in underdoped samples, is the only one present, then describing superconductivity as arising from the condensation of pre-formed pairs as in the model considered here is quite appealing. In this respect, we should comment on a recent suggestion$^{21}$ that the spin gap in the attractive model may be irrelevant to the cuprates, as the observed suppression of the uniform susceptibility would be due solely to antiferromagnetic fluctuations. It may be possible to reconcile both views if one considers a Hubbard model with on-site repulsion and nearest-neighbor attraction. In this case, the superconducting phase is near a spin-density wave (SDW) instability$^6$, and SDW fluctuations could influence the magnetic response as suggested. Moreover, the superconducting order parameter in that region has been predicted$^6$ to have $d$-wave symmetry, in agreement with penetration depth$^{22}$, and photoemission$^{23}$ studies. Work is in progress to test these ideas.

**ACKNOWLEDGMENTS**

The author is grateful to M. A. Continentino for useful discussions. Financial support from the Brazilian Agencies MCT, CNPq, and CAPES is also gratefully acknowledged.

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