Quantum Transition between an Antiferromagnetic Mott Insulator and $d_{x^2-y^2}$ Superconductor in Two Dimensions

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We consider a Hubbard model on a square lattice with an additional interaction, W, which depends upon the square of the near-neighbor hopping. At half filling and a constant value of the Hubbard repulsion, increasing the strength of the interaction W drives the system from an antiferromagnetic Mott insulator to a $d_{x^2-y^2}$ superconductor. This conclusion is reached on the basis of zero temperature quantum Monte Carlo simulations on lattice sizes up to 16×16. [S0031-9007(96)01756-5]

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At half filling, the two-dimensional (2D) Hubbard model on a square lattice with a near-neighbor one-electron hopping t and an on-site Coulomb interaction U has an insulating ground state with long-range antiferromagnetic (AF) order. When carriers are doped into this insulating state, the possibility of a transition to a $d_{x^2-y^2}$ superconducting state has been extensively pursued. However, at energy scales and lattice sizes accessible to numerical simulations of the 2D Hubbard model, no definite sign of superconductivity has been found in the vicinity of the Mott transition [1]. An alternate approach for studying the transition from the Mott insulator to a $d_{x^2-y^2}$ superconducting state is to keep the system at half filling, but add an interaction which can drive the system into a $d_{x^2-y^2}$ superconducting ground state. Here, we introduce a simple form for such an interaction which depends on the square of a near-neighbor hopping. We note that it can formally be obtained from a Su-Schrieffer-Heeger [2] interaction in the antiadiabatic limit. It may also be viewed as derived from purely electronic origins near the AF Mott insulator. However, our purpose is not aimed at describing the pairing mechanism but rather at studying the transition between an antiferromagnetic Mott insulating state and a $d_{x^2-y^2}$ superconducting state. In this sense, we view the interaction as a formal way of obtaining a model which exhibits this transition and is suitable for Monte Carlo simulations in that there are no fermion sign problems.

The basic half-filled Hubbard model that we will study has the Hamiltonian,

$$H_U = -\frac{t}{2}\sum_{\vec{i}} K_{\vec{i}} + U\sum_{\vec{i}}(n_{\vec{i},\uparrow} - \tfrac{1}{2})(n_{\vec{i},\downarrow} - \tfrac{1}{2}), \quad (1)$$

with the hopping kinetic energy,

$$K_{\vec{i}} = \sum_{\sigma,\vec{\delta}}(c^{\dagger}_{\vec{i},\sigma}c_{\vec{i}+\vec{\delta},\sigma} + c^{\dagger}_{\vec{i}+\vec{\delta},\sigma}c_{\vec{i},\sigma}). \quad (2)$$

Here, $c^{\dagger}_{\vec{i},\sigma}$ ($c_{\vec{i},\sigma}$) creates (annihilates) an electron with a z component of spin σ on-site $\vec{i}$, $n_{\vec{i},\sigma} = c^{\dagger}_{\vec{i},\sigma}c_{\vec{i}\sigma}$, and $\vec{\delta} = \pm\vec{a}_x, \pm\vec{a}_y$, where $\vec{a}_x$, $\vec{a}_y$ are the lattice constants. The energy will be measured in units of t. The interaction that we will add has the following form:

$$H_W = -W\sum_{\vec{i}} K^2_{\vec{i}}, \quad (3)$$

with positive W. We note that the interaction H_W can be generated from a Su-Schrieffer-Heeger [2] term with Einstein oscillators:

$$\sum_{\langle\vec{i},\vec{j}\rangle,\sigma}\vec{\lambda}\cdot\left(\vec{Q}_{\vec{i}} - \vec{Q}_{\vec{j}}\right)\left(c^{\dagger}_{\vec{i},\sigma}c_{\vec{j},\sigma} + \text{H.c.}\right) + \sum_{\vec{i}}\left(\frac{\vec{P}^2_{\vec{i}}}{2M} + \vec{Q}_{\vec{i}}{}^{\dagger}\frac{D}{2}\vec{Q}_{\vec{i}}\right). \quad (4)$$

Integrating out the phonons and taking the antiadiabatic limit ($M \to 0$) generates H_W with $W = \vec{\lambda}^{\dagger}D^{-1}\vec{\lambda}/2$. Pairing mechanisms along those lines were considered in [3,4]. This derivation should be compared to the case of the attractive Hubbard model which may be obtained in a similar way provided that electron-phonon interaction is chosen to be of the Holstein form [5]. In fact, one of the reasons for choosing this form is that it has a simple Hubbard-Stratonovitch representation which is useful in constructing the Monte Carlo simulation.

The Hamiltonian

$$H = H_U + H_W \quad (5)$$

has the possibility of exhibiting a quantum transition between an AF Mott insulating state and a superconducting phase. When $W = 0$, the half-filled Hubbard model with a finite U is known to be a Mott insulator with long-range AF order. The interaction H_W can be decomposed into single-particle next-nearest-neighbor hopping terms, singlet pair-hopping terms involving on-site singlet pairs, triplet pair-hopping processes, and terms of the form,

$$-W\sum_{\vec{i},\vec{\delta},\vec{\delta}'}(\Delta^{\dagger}_{\vec{i},\vec{\delta}'}\Delta_{\vec{i},\vec{\delta}} + \text{H.c.}), \quad (6)$$

where $\Delta^{\dagger}_{\vec{i},\delta} = (c^{\dagger}_{\vec{i},\uparrow}c^{\dagger}_{\vec{i}+\vec{\delta},\downarrow} - c^{\dagger}_{\vec{i},\downarrow}c^{\dagger}_{\vec{i}+\vec{\delta},\uparrow})/\sqrt{2}$. In the presence of the Hubbard Hamiltonian, H_U, the latter term (6)

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dominates the low energy physics, and, as we will see, leads to a $d_{x^2-y^2}$ superconducting state.

We have carried out our simulations with a zero temperature quantum Monte Carlo (QMC) algorithm [6,7]. At half filling the Hamiltonian, Eq. (5), is particle-hole symmetric at any U and W so that there is no sign problem and ground state simulations on *large* lattices (up to 16×16) were carried out without any complications. This statement is valid even for twisted boundary conditions for which

$$c^{\dagger}_{\vec{i}+L\vec{a}_x,\sigma} = \exp(2\pi i \Phi/\Phi_0) c^{\dagger}_{\vec{i},\sigma} \quad \text{and} \quad c^{\dagger}_{\vec{i}+L\vec{a}_y,\sigma} = c^{\dagger}_{\vec{i},\sigma}\,, \tag{7}$$

with $\Phi_0 = hc/e$ the flux quanta and L the linear length of the square lattice. The boundary conditions given by Eq. (7) account for a magnetic flux threading a torus on which the lattice is wrapped. To take advantage of the efficiency of a single spin-flip algorithm, we have carried out a discrete Hubbard-Stratonovitch transformation of the H_W term. The transformation produces an overall systematic error of order $(\Delta\tau W)^3$, where $\Delta\tau$ corresponds to the imaginary time step entering the path integral formulation. This systematic error is negligible compared to the one produced by the Trotter decomposition which is of order $(\Delta\tau)^2$. Unless mentioned otherwise, we have carried out our simulations at $\Delta\tau t = 0.0625$. The details of the algorithm will be presented elsewhere [8].

We first concentrate on the charge degrees of freedom with $U/t = 4$, and study the ground state as a function of W/t. In order to do so, we have computed the ground state energy as a function of the twist in the boundary condition, $E_0(\Phi)$. For an insulator, the wave function is localized, and, hence, an exponential decay of $\Delta E_0(\Phi) \equiv E_0(\Phi) - E_0(\Phi_0/2)$ as a function of lattice size is expected [9]. In the spin density wave (SDW) approximation for the half-filled Hubbard model, one obtains $\Delta E_0(\Phi) = \alpha(\Phi) L \exp(-L/\xi)$, where ξ is the localization length of the wave function. On the other hand, for a superconductor, $\Delta E_0(\Phi)$ shows anomalous flux quantization: $\Delta E_0(\Phi)$ is a periodic function of Φ with period $\Phi_0/2$, and a nonvanishing energy barrier is to be found between the flux minima [10–12] so that $\Delta E_0(\Phi_0/4)$ remains finite as $L \to \infty$. Figure 1(a) shows $\Delta E_0(\Phi_0/4)$ versus $1/L$ for various values of W/t. One observes a change in the size scaling of $\Delta E_0(\Phi_0/4)$ as W/t decreases from $W/t = 0.5$ to $W/t = 0.22$. From these measurements, we estimate that the change occurs in the vicinity of $W/t = 0.3$. For values of $W/t < 0.3$, $\Delta E_0(\Phi_0/4)$ is consistent with the SDW form, whereas, for $W/t \geq 0.33$, $\Delta E_0(\Phi_0/4)$ may be fitted to a $1/L$ form and scales to a finite value. The extrapolated value of $\Delta E_0(\Phi_0/4)$ versus W/t is plotted in Fig. 1(b), and the quantum transition between a Mott insulator and superconductor occurs at $W/t \sim 0.3$.

In order to determine the symmetry of the order parameter in the superconducting state, we have calculated

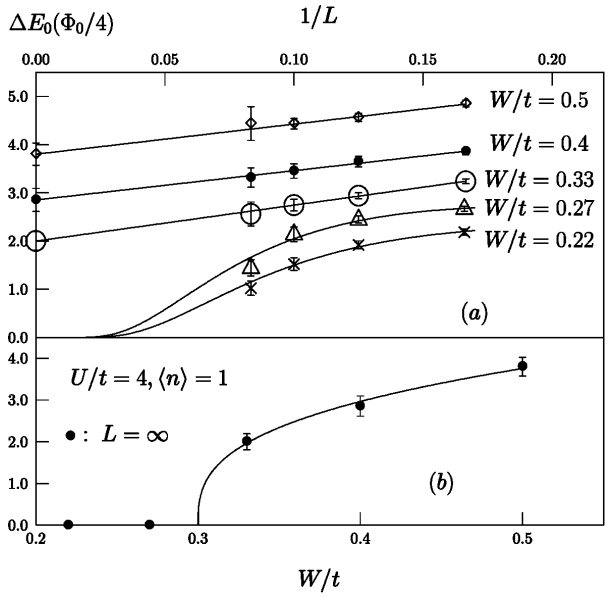

FIG. 1. (a) $\Delta E_0(\Phi_0/4) \equiv E_0(\Phi_0/4) - E_0(\Phi_0/2)$ versus $1/L$ for several values of W/t. For $W/t < 0.3$ the solid lines correspond to a least squares fit of the data to the SDW form, $L\exp(-L/\xi)$. For $W/t > 0.3$ the QMC data is compatible with a $1/L$ scaling. The solid lines are least squares fits to this form. (b) Extrapolated value of $\Delta E_0(\Phi_0/4)$ versus W/t. The solid line is a guide to the eye.

pair-field correlations in the s and $d_{x^2-y^2}$ channels:

$$P_{d,s}(\vec{r}) = \langle \Delta^{\dagger}_{d,s}(\vec{r}) \Delta_{d,s}(\vec{0}) \rangle\,, \tag{8}$$

with

$$\Delta^{\dagger}_{d,s}(\vec{r}) = \sum_{\sigma,\vec{\delta}} f_{d,s}(\vec{\delta}) \sigma c^{\dagger}_{\vec{r},\sigma} c^{\dagger}_{\vec{r}+\vec{\delta},-\sigma}\,. \tag{9}$$

Here, $f_s(\vec{\delta}) = 1$ and $f_d(\vec{\delta}) = 1(-1)$ for $\vec{\delta} = \pm\vec{a}_x$ $(\pm\vec{a}_y)$. Figure 2 shows plots of $P_{d,s}(L/2, L/2)$ for $W/t = 0.6$ where the system is superconducting, and $W/t = 0.1$ where it is not. At $W/t = 0.6$, the dominant signal at long distances ($L = 16$) is obtained in the $d_{x^2-y^2}$ channel.

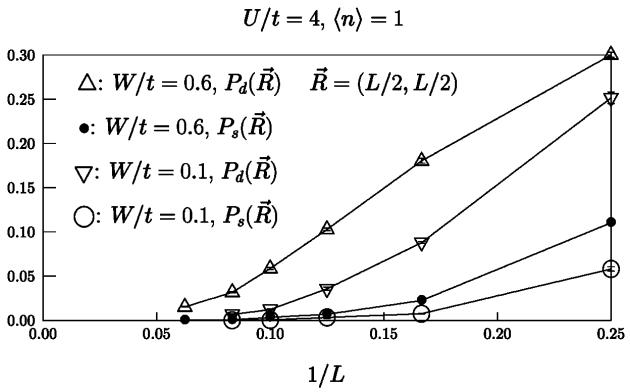

FIG. 2. $d_{x^2-y^2}$ (triangles) and s-wave (circles) pair-field correlations versus $1/L$.

At the mean-field level, the symmetry of the order parameter will determine the functional form of the single-particle occupation number, $n(\vec{k})$. For a $d_{x^2-y^2}$ superconductor the BCS result yields

$$n(\vec{k}) = 1 + \frac{\epsilon_{\vec{k}}}{\sqrt{\Delta_{\vec{k}}^2 + \epsilon_{\vec{k}}^2}}, \tag{10}$$

where $\epsilon_{\vec{k}} = -2t[\cos(k_x) + \cos(k_y)]$ and $\Delta_{\vec{k}} = \Delta_0[\cos(k_x) - \cos(k_y)]$. As apparent from Eq. (10) in the $\vec{k} = k(1,1)$ direction the $d_{x^2-y^2}$ gap vanishes, and $n(\vec{k})$ shows a jump at the Fermi energy, whereas in the $\vec{k} = k(1,0)$ direction $n(\vec{k})$ is a smooth function of k. Precisely this behavior in $n(\vec{k})$ may be detected in the QMC data at $W/t = 0.6$ as shown in Fig. 3(a). For comparison, we have plotted $n(\vec{k})$ at $W = 0$, where it is expected to scale to a smooth function in the thermodynamic limit [see Fig. 3(b)].

We now consider the spin degrees of freedom. We have computed the real space spin-spin correlations,

$$S(\vec{r}) = \tfrac{4}{3}\langle \vec{S}(\vec{r})\vec{S}(\vec{0})\rangle, \tag{11}$$

where $\vec{S}(\vec{r})$ is the spin operator at site $\vec{r}$. For values of $W/t < 0.3$ and lattice sizes ranging from $L = 4$ to $L = 12$, $S(L/2, L/2)$ may be fitted to a $1/L$ form and scales to a finite value, as shown in Fig. 4(a). We therefore conclude that long-range AF order is present for $W/t < 0.3$. The associated staggered moment, $m = \lim_{L\to\infty}\sqrt{3S(L/2, L/2)}$, is plotted in Fig 4(b). The data is consistent with a continuous decay of m as W/t increases towards 0.3. At $W/t = 0.3$, we were unable to distinguish m from zero within our statistical uncertainty. Hence, we conclude that long-range AF order vanishes at $W/t \sim 0.3$. Therefore, within our numerical resolution, the antiferromagnetic transition point is not separated from the superconductor-insulator transition point. Well within the $d_{x^2-y^2}$ superconducting phase the spin-spin correlations remain sizable. In fact, at $W/t = 0.6$, lattice sizes ranging from $L = 4$ to $L = 16$, $S(L/2, L/2)$ scales as $L^{-\alpha}$ with $\alpha = 1.16 \pm 0.01$ as shown in the inset of Fig. 4(a). This slow decay of the spin-spin correlations in the superconducting state arises because of the nodes in the $d_{x^2-y^2}$ gap. Following Ref. [13], one can approximate the spin susceptibility, $\chi(\vec{q}, i\omega_m)$, in the superconducting state by inserting the irreducible BCS spin susceptibility, $\chi_0(\vec{q}, i\omega_m)$, in the random phase approximation (RPA) form of $\chi(\vec{q}, i\omega_m)$: $\chi_{\mathrm{RPA}}(\vec{q}, i\omega_m) = \chi_0(\vec{q}, i\omega_m)/[1 - U\chi_0(\vec{q}, i\omega_m)]$. Here, ω_m corresponds to Matsubara frequencies. Within this approximation and at half-band filling, the spin-spin correlations for a $d_{x^2-y^2}$ superconducting order parameter show a power-law decay. In contrast, for an s-wave order parameter, an exponential decay is obtained.

We have found a simple model, Eq. (5), which exhibits a ground state transition from an AF Mott insulator to a $d_{x^2-y^2}$ superconductor. Specifically, for $U/t = 4$ at half filling ($\langle n\rangle = 1$) we have found that this transition occurs at $W_c \sim 0.3t$. As a natural consequence of these results, we expect, for values of $W < W_c$, the occurrence of a quantum transition between an AF Mott insulator and a $d_{x^2-y^2}$ superconductor as a function of chemical

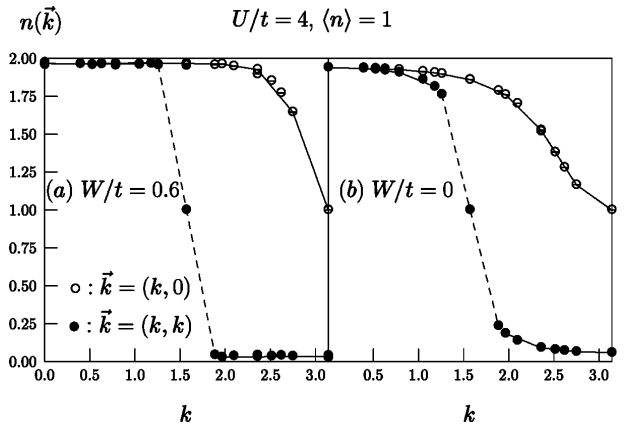

FIG. 3. (a) $n(\vec{k})$ at $W/t = 0.6$, $U/t = 4$, and $\langle n\rangle = 1$. Lattices from $L = 8$ to $L = 16$ were considered; (b) same as (a) but for $W/t = 0$. The calculations in this figure were carried out at $\Phi = 0$ [see Eq. (7)].

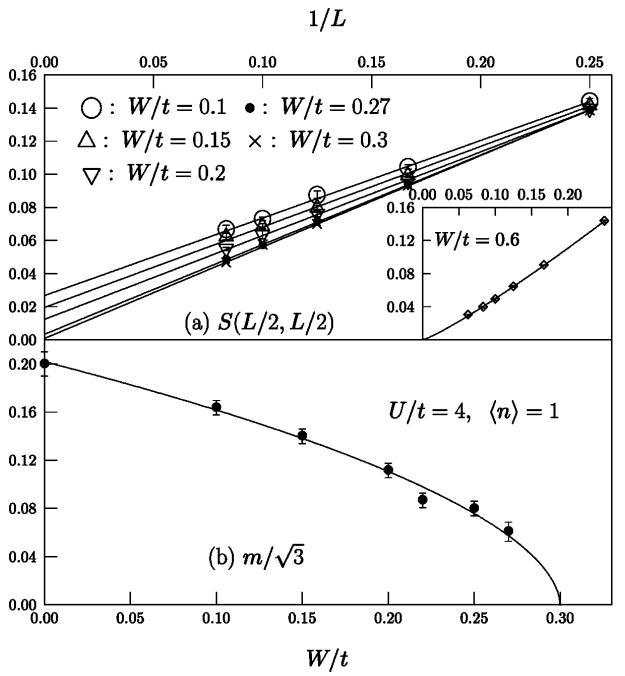

FIG. 4. (a) $S(L/2, L/2)$ versus $1/L$ for several values of W/t. The solid lines correspond to least squares fits of the QMC data to the form $1/L$. Inset: $S(L/2, L/2)$ versus $1/L$ at $W/t = 0.6$. The solid is a least squares fit to the form $L^{-\alpha}$. (b) Staggered moment as obtained from (a) versus W/t. The data point at $W/t = 0$ is taken from Ref. [14]. At $W/t = 0.3$, we were unable to distinguish m from zero within our statistical uncertainty. The solid line is a guide to the eye. The calculations in this figure were carried out at $\Phi = 0$ [see Eq. (7)].

potential μ. It has recently been concluded that, for the 2D Hubbard model ($W = 0$), the quantum transition between the AF Mott insulator and metallic state driven by the chemical potential belongs to a universality class characterized by an unusually large dynamical exponent, $z = 4$ [15–17]. The presence of the H_W term may bypass this suppression of coherence observed at $W = 0$ and introduce another independent energy scale to drive the Mott transition. At constant U and in the W, μ plane, the Hamiltonian (5) is expected to lead to a rich structure of quantum transitions involving the Mott insulating state, the d-wave superconducting state and metallic states as well as crossovers at finite temperatures. Although the justification of the model from a microscopic point of view is at present uncertain, it provides us with a model to study some of the salient ground state and finite temperature features of a $d_{x^2-y^2}$ superconductor at an energy scale accessible to numerical simulations. It also allows us to study a quantum transition between an AF Mott insulator and a $d_{x^2-y^2}$ superconductor.

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Note added.—Although the QMC data of Fig. 3(b) supports a continuous decay of the staggered moment, we cannot exclude the possibility that the quantum transition is of weakly first order as would be the case in a mean-field approach. D. J. S. thanks S. Kivelson for raising this issue.

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