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Energetics of superconductivity in the two-dimensional Hubbard model

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The energetics of the interplay between superconductivity and the pseudogap in high-temperature superconductivity is examined using the eight-site dynamical cluster approximation to the two-dimensional Hubbard model. Two regimes of superconductivity are found: a weak-coupling/large-doping regime in which the onset of superconductivity causes a reduction in potential energy and an increase in kinetic energy, and a strong-coupling regime in which superconductivity is associated with an increase in potential energy and a decrease in kinetic energy. The crossover between the two regimes is found to coincide with the boundary of the normal-state pseudogap, providing further evidence of the unconventional nature of superconductivity in the pseudogap regime. However, the absence, in the strongly correlated but nonsuperconducting state, of discernibly nonlinear response to an applied pairing field suggests that resonating valence bond physics is not the origin of the kinetic-energy driven superconductivity.

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The high transition temperature superconductivity exhibited by layered copper-oxide materials has been an important topic in condensed-matter physics since its discovery in 1986.[1] Broadly speaking, two views are currently held. One is that despite the various anomalous features of the materials the superconductivity may be understood in more or less conventional Bardeen-Cooper-Schrieffer (BCS) terms as arising from the exchange of a pairing ("glue") particle, most likely of magnetic origin.[2] An alternate view is that the superconductivity is an intrinsic property of a strongly correlated state of matter that should not be interpreted as arising from the exchange of a well-defined excitation.[3]

The issue may be cast in energetic terms. In the conventional BCS view, the driving force for superconductivity is in essence a reduction of potential energy: by forming the superconducting state the electrons can take greater advantage of an attractive term in an interparticle potential. Changing the wave function to reduce the potential energy, however, costs kinetic energy, so that in the weak-coupling limit the change from normal to superconducting states leads to an increase in the kinetic energy.[4] In an alternate view,[3] the driving force for superconductivity is an optimization of kinetic energy: by forming the superconducting state the electrons can move more easily through the crystal despite their need to avoid the other electrons. In this case going from the normal to the superconducting state lowers the kinetic energy and one expects that the potential energy increases.

The repulsive-U Hubbard model on the two-dimensional square lattice is widely believed[3,5,6] to contain the essential physics of high-T_c copper-oxide superconductivity. It is defined by the Hamiltonian

$$H = \sum_{k\sigma}(\varepsilon_k - \mu)c^\dagger_{k\sigma}c_{k\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}. \quad (1)$$

Here i labels the sites in a lattice and k a momentum in the corresponding Brillouin zone. The two-dimensional repulsive ($U > 0$) version of the model has been shown rigorously to have a $d_{x^2-y^2}$ superconducting ground state in at least some regions of the U,n phase diagram.[7–9]

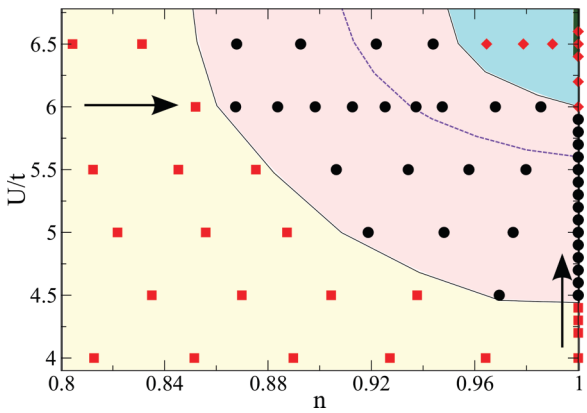

FIG. 1. (Color online) Phase diagram of two-dimensional square lattice Hubbard model in plane of density n and interaction strength U/t at inverse temperature $\beta = 60/t$ as obtained in eight-site cluster dynamical mean-field theory. Mott insulator at half filling for $U/t \gtrapprox 6.4$ indicated by heavy bar (green online); superconducting region indicated by circles (black online), pseudogapped but nonsuperconducting region, diamonds (blue online) and Fermi-liquid nonsuperconducting state by squares (yellow online). Boundary of normal-state pseudogap, defined as in Ref. 10, indicated as dashed line (purple online). Trajectories along which the energy is computed are shown as arrows.

In this paper we investigate the electronic energy $E = \langle H\rangle$, decomposed into kinetic K and potential V terms as $E = K + V$ with

$$K = \sum_{k\sigma}\varepsilon_k\langle c^\dagger_{k\sigma}c_{k\sigma}\rangle = 2T\sum_{k,n}(\varepsilon_k - \mu)\mathrm{Tr}[\tau_3 G(k,\omega_n)], \quad (2)$$

$$V = U\sum_i\langle n_{i\uparrow}n_{i\downarrow}\rangle = 2T\sum_{k,n}\mathrm{Tr}[\Sigma(k,\omega_n)G(k,\omega_n)]. \quad (3)$$

In the second equality we have used standard formulas to reexpress the expectation values in terms of the Nambu matrix Matsubara frequency electron Green function G and self-energy Σ.

The energetics of superconductivity have been previously studied. One important class of approaches has used variational

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wave functions, often starting from a single Slater determinant with doubly occupied sites then being projected out.[11–18] Information about pairing comes from comparing results obtained from free fermion and BCS-paired starting points. These works indicated that pairing was present for dopings from $x = 0$ to $x \sim 0.25$ and that over most of the phase diagram the kinetic energy of the paired state was lower than that of the unpaired state. However, variational results are constrained by the choice of variational space; in particular by the choice of projective BCS-type wave functions.

Another important class of theoretical approaches involves phenomenological spin-fermion models.[19–25] In these approaches it is assumed that the important physics arises from the interaction of electrons with spin fluctuations (treated as bosons but with boson self-energy effects arising from coupling to fermions playing a crucial role). These models are amenable to semianalytic treatment. Their analysis revealed that in the strong-coupling limit the superconducting state could have lower kinetic energy than the normal state. However, these models do not fully capture the strong correlation effects associated with the Mott transition or the formation of the pseudogap, and rely on assumptions about the most physically relevant interactions.

We use the dynamical cluster approximation (DCA) version of dynamical mean-field theory[26] to evaluate Eqs. (2) and (3) for the two-dimensional repulsive-U Hubbard model with $\varepsilon_k = -2t(\cos k_x + \cos k_y)$. In the DCA the Brillouin zone is tiled with N patches and the electron self-energy is taken to be piecewise constant, with a different value in each sector of momentum space. The sector self-energies are obtained from the solution of an auxiliary quantum impurity model with parameters fixed by the Hubbard interaction and a self-consistency condition discussed in detail in Ref. 26. The method yields a $d_{x^2-y^2}$ superconducting state.[5,27–38] For the Hubbard model the method becomes exact as $N \to \infty$ and considerable evidence is now available[39–42] concerning the status of the finite N results achievable numerically. Here we study the case $N = 8$, which has been shown to be large enough for the results to be representative of the infinite cluster size limit[9] but small enough to enable calculations of the necessary accuracy.[40]

We obtained the superconducting kinetic and potential energies KE_S and PE_S from superconducting solutions obtained as described in Ref. 38 and the normal-state energies KE_N and PE_N by solving the DMFT equations in the paramagnetic phase with the same code but subject to the constraint that the anomalous ($\langle cc \rangle$) terms in the Green function and self-energy vanished. Our results are obtained using the CT-AUX version[43] of the continuous-time quantum Monte Carlo method[44] with submatrix updates[45] and an extension to superconductivity.[38] The energy differences are found to be very small and careful attention to the high-frequency behavior is required for reliable results. The submatrix methods are essential in obtaining data of the requisite accuracy.

Figure 1 shows the phase diagram obtained from the $N = 8$ DCA method in the interaction strength and doping plane[38] along with two arrows indicating the parameter-space trajectories along which energies are computed in this paper. At $U \gtrsim 6.4t$ and carrier concentration $n = 1$ per site the approximation yields a paramagnetic ("Mott") insulating state which is at lower temperatures unstable to antiferromagnetism. As electrons are removed the state evolves to a conventional Fermi-liquid metal via an intermediate "strange metal" phase characterized by a "pseudogap," a suppression of electronic density of states in the $(0,\pi)$ region of the Brillouin zone.[10,40,46–54] Superconductivity is found in a strip,[38] near the Mott insulator but separated from it by a region of pseudogapped but nonsuperconducting states.[53] At carrier concentration $n = 1$ (vertical arrow) the ground state of the model is believed to be antiferromagnetic at all U. The $n = 1$ results were obtained by suppressing long-ranged antiferromagnetic order (although short-ranged antiferromagnetic correlations are still present) and are representative of the properties of a metastable state. They are included because the qualitative properties are seen to be the same as in the doping-driven transition but the particle-hole symmetry at $n = 1$ permits the acquisition of much higher quality data, enabling a clearer view of the phenomena.

The two panels of Fig. 2 show the energy differences obtained by subtracting the superconducting and normal-state energies computed at inverse temperature $\beta = 60/t$ along the two parameter-space trajectories shown by the arrows in Fig. 1, i.e., crossing the superconducting region by varying the interaction strength or varying the carrier concentration. The results obtained along the two trajectories are remarkably similar, although the absence of a fermion sign problem at $n = 1$ means we are able to obtain much better statistics in this

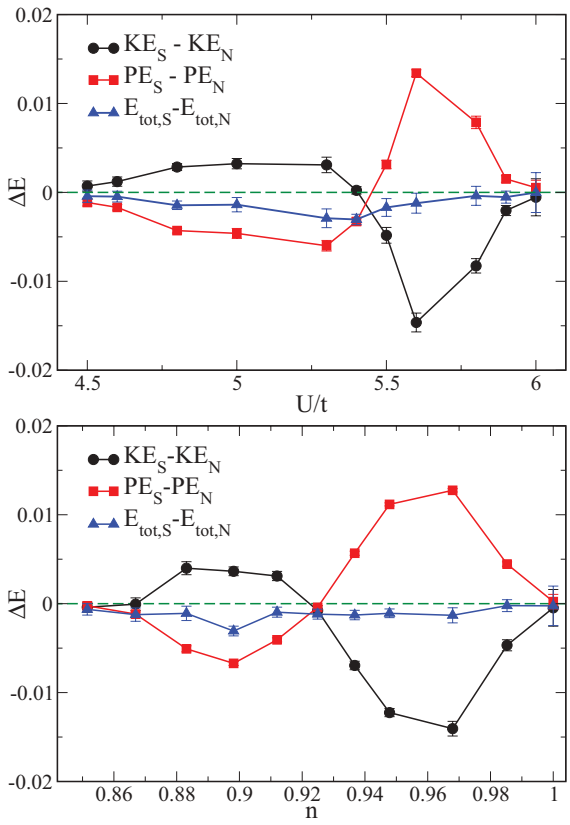

FIG. 2. (Color online) Differences in total, kinetic, and potential energies (per site, in units of hopping t) between normal and superconducting states, obtained as described in the text at density $n = 1$ varying interaction strength (upper panel) and as function of density at fixed interaction strength $U = 6t$ (lower panel).

case. The condensation energy is of order $0.001t$, although the changes in kinetic and potential energy separately are typically much larger, especially in the pseudogap regime.

For interactions or carrier concentrations smaller than required to produce a normal-state pseudogap,[10,40,49] the energetics are consistent with the standard expectations of weak-coupling superconductivity: as the material enters the superconducting state the potential energy decreases and the kinetic energy increases. The boundary of the normal-state pseudogap marks a significant change in the energetics of superconductivity: once the pseudogap regime is entered, the kinetic energy decreases and the potential energy increases on entering the superconducting state. Further, inside the pseudogap regime the superconducting/normal changes in potential and kinetic energy become much larger in magnitude, showing that the onset of superconductivity leads to a significant re-organization of the energetics of the pseudogap states. The change in character of the superconductivity at the pseudogap line is consistent with the finding of Yang *et al.*[53] that the superconductivity exists in a dome with the maximal transition temperature occurring where the superconducting and pseudogap phase boundaries intersect. The change is also consistent with the finding of Kyung *et al.*[55] that the pseudogap is associated with a decrease in the pairing potential.

Our results differ from previous dynamical mean field analyses. Reference 56 ($N = 4$ study of the Hubbard model) found that both at low and high doping superconductivity was associated with a decrease in kinetic energy, with negligible changes in potential energy. Reference 57 ($N = 4$ study of the t-J model, with an additional "EDMFT" approximation) found that most of the energy gain on entering the superconducting state came from changes in the interaction term, although the behavior of the kinetic energy was different at large than at small doping. Three possible origins for the discrepancy are the use of the noncrossing approximation ("NCA") impurity solver in Refs. 56 and 57 rather than the numerically exact CT-QMC method, the use of the $N = 4$ approximation, rather than the $N = 8$ approximation used here, and the study of the t-J rather than Hubbard model in Ref. 57. Singh[58] has questioned the relevance of computations based on the t-J model, because of apparent violations of the virial theorem which may be traced back to the fact that some parts of the electron kinetic energy are included in the "J" coupling.

The "potential-energy driven" nature of the superconductivity found at larger dopings and at weak couplings is consistent with the notion that in these regimes the superconductivity is relatively conventional. The change in energetics as the pseudogap boundary is crossed suggests that at stronger couplings or lower dopings the superconductivity becomes unconventional. One influential model of unconventional superconductivity is the resonating valence bond (RVB) idea of Anderson[3] which was motivated in part by the possibility that the physics of the cuprates could be understood in terms of a very-strong-coupling limit of the Hubbard model. There, configurations with two electrons on a site could be projected out so that the only important term in the energy was the kinetic-energy term and superconductivity (and indeed all other interesting physics) is necessarily "kinetic-energy driven."

Anderson's original RVB idea, and subsequent recognition of an SU(2) symmetry in the RVB wave function which might

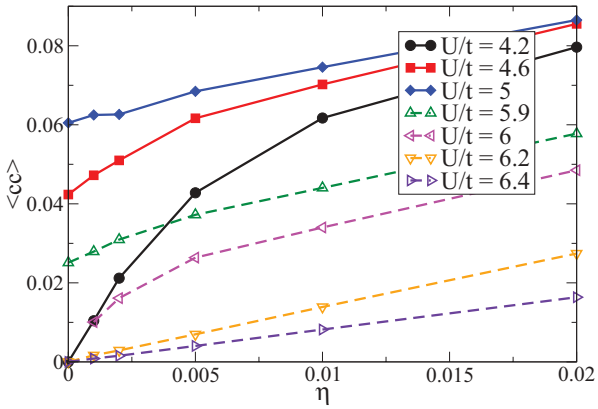

FIG. 3. (Color online) Anomalous expectation value in sector $K = (0,\pi)$ plotted against pairing field η at doping $x = 0$ for interaction strengths indicated.

be weakly broken by doping or small finite U corrections[59] implied that superconducting correlations were present (but not active) in the Mott insulating state and the strongly correlated but not superconducting state which separates the superconducting and insulating regimes in Fig. 1. To test this hypothesis we applied a pairing field $\eta_K(c^\dagger_{K\uparrow}c^\dagger_{K\downarrow} + c_{K\uparrow}c_{K\downarrow})$ in our calculations and computed the effect on the superconducting order parameter $\langle c_{K\uparrow}c_{K\downarrow}\rangle$. We expect that if a near-SU(2) symmetry existed, then applying a small pairing field to a state which is nonsuperconducting but is near the phase boundary would provide a rapid increase in the pairing amplitude, which would then saturate to a value characteristic of the superconducting state. Figure 3 shows that this is not the case. On the weak-coupling side ($U = 4.2$), applying a pairing field leads to the behavior expected near a second-order phase transition: a rapid increase in $\langle cc\rangle$ reflecting the enhanced susceptibility, followed by a saturation to values similar to those found in the nearby superconducting state. However, on the strong-coupling side the situation is different. Just at the phase boundary $U = 6.0$ the situation is similar to that found at weak coupling, but for any larger U the $\langle cc\rangle$ vs η curve is linear with small, weakly U-dependent slope. The similarity of the $U = 6.2$ and 6.4 results, and the difference of both of these to the $U = 4.2$ trace, indicates that precursor effects are very weak as the superconducting phase is approached from the pseudogap indicating that the pseudogap state has no strong tendency towards superconductivity. We infer from this calculation that the origin of the kinetic-energy driven behavior is not a signature of pairing correlations pre-existing in the wave function.

It is interesting to consider the normal-superconducting energy differences in the context of the energetics of the pseudogap state itself. The two panels of Fig. 4 show the temperature dependence of the kinetic energy computed for a relatively weak coupling, $U = 5.0t$ (lower panel) and relatively strong coupling, $U = 5.8t$ (upper panel). We see that in the weak-coupling case, the kinetic energy decreases as the temperature is lowered, and the onset of superconductivity reverses this decrease, while in the strongly coupled case the kinetic energy increases as temperature is lowered but the onset of superconductivity again reverses the temperature dependence.

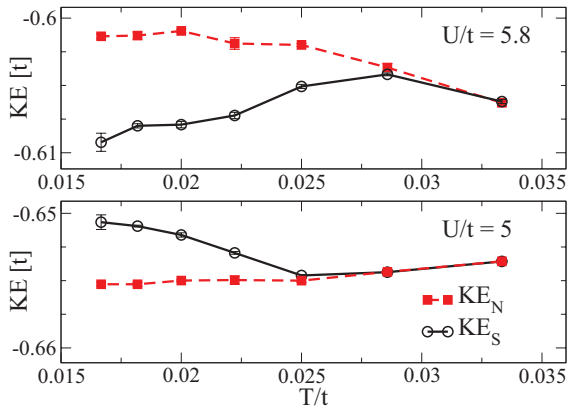

FIG. 4. (Color online) Temperature dependence of kinetic energy at $n = 1$ for $U = 5.0$ (lower panel) and $U = 5.8$ (upper panel) in normal (filled squares, red dashed line) and superconducting state (open circles, black solid line).

We finally consider the observability of these effects. Norman and co-workers noted that the difference between normal-state and superconducting state photoemission spectra could be analyzed to obtain estimates of the normal-superconducting change both in total and in kinetic energy[60] although the analysis is complicated by the need to accurately monitor small changes occurring over wide energy and momentum ranges. Specific-heat data can also be used to infer the condensation energy, although care must be taken both to extrapolate the normal state to temperatures less than the transition temperature and to include fluctuation effects.[61] In narrow-band systems such as cuprates, an approximate relation between the kinetic energy and the frequency integral of the optical conductivity exists.[62–64] Interestingly the idea of examining superconductivity-induced changes in the optical integral seems to have entered the high-T_c literature first in the context of the "hole superconductivity" model of Hirsch[65,66] and then by Chakravarty and collaborators[67] in relation to the interlayer coherence mechanism of Anderson.[68] These works motivated several experimental groups to examine changes in optical conductivity across the normal-superconducting phase boundary.[69–73] Unfortunately, the value of the optical spectral weight depends on the frequency up to which the conductivity is integrated, and the appropriate upper cutoff may be different in the normal and superconducting state;[23,24] also even if the conduction-band contribution to the optical sum rule could be determined, the relation between this and the kinetic energy is only approximate, and the errors involved in the approximation may be different in the normal and superconducting state.[25] As can be seen from Fig. 4, the temperature-dependent changes are only on the 1% level.

In summary, our results indicate that the nature of the superconductivity depends crucially on location in the phase diagram. For the high doping/weak correlation side of the superconducting region, the energetics of superconductivity appear essentially conventional: on transition to the superconducting state the potential energy decreases and the kinetic energy increases. On the low doping/strong correlation side of the superconducting region, the energetics appears unconventional: on entering the superconducting state the kinetic energy decreases and the potential energy increases. However, we do not find any indication that the nonsuperconducting pseudogap state has any significant pairing correlations, casting doubt on an RVB interpretation of the pseudogap. Interestingly, the crossover between the two regimes occurs essentially at the point at which the pseudogap becomes visible in normal-state quantities and also interestingly the changes in the individual components of the energy become much larger in this unconventional regime, suggesting that superconductivity causes a substantial rearrangement of the pseudogap electronic state. In other words, the superconductivity and pseudogap are competing phases.

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