Kinetic Energy Driven Pairing in Cuprate Superconductors

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Pairing occurs in conventional superconductors through a reduction of the electronic potential energy accompanied by an increase in kinetic energy. In the underdoped cuprates, optical experiments show that pairing is driven by a reduction of the electronic kinetic energy. Using the dynamical cluster approximation we study superconductivity in the two-dimensional Hubbard model. We find that pairing is indeed driven by the kinetic energy and that superconductivity evolves from an unconventional state with partial spin-charge separation, to a superconducting state with quasiparticle excitations.

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The theory of superconductivity in the cuprates remains one of the most important outstanding problems in materials science. Conventional superconductors are well described by the Bardeen-Cooper-Schrieffer (BCS) theory. Here, the transition is due to the potential energy that electrons can gain by forming Cooper pairs. However, recent optical experiments show that the transition in the cuprates is due to a lowering of the electronic *kinetic* energy, suggesting that the mechanism for superconductivity in the cuprates is unconventional.

In the BCS theory, pairing is a result of a Fermi surface instability that relies on the existence of quasiparticles in a Fermi liquid. The electrons interact by exchanging phonons leading to a net attractive force between them. In the BCS reduced Hamiltonian, the phonon-mediated interaction is represented by an attractive pairing potential, and the system can lower its potential energy by forming pairs which have s-wave symmetry due to the local nature of the pairing interaction. To take full advantage of this energy reduction, the electrons forming the pair have to occupy states outside the Fermi sea with an energy above the Fermi energy. As a result, pairing in conventional superconductors is always associated with an increase in the electronic kinetic energy [1] which is overcompensated by the lowering of the electronic potential energy.

High-temperature cuprate superconductors (HTSC) are unconventional in various aspects and the pairing mechanism remains controversial. The HTSC emerge from their antiferromagnetic parent compounds upon hole doping. The normal state of the weakly doped cuprates is not a Fermi liquid, undermining the very foundation of BCS theory. It is widely believed that phonons cannot be responsible for pairing at temperatures as high as 160 K. Consistently, the pairs have d-wave, instead of s-wave symmetry. By analyzing photoemission data Norman *et al.* pointed out the possibility of kinetic energy driven pairing in the underdoped cuprates [2]. Most significantly, new optical experiments [3,4] confirm this conjecture. These experiments show that pairing in high-temperature superconductors is driven by a reduction of the kinetic energy, not by an attractive potential as in the BCS theory, and therefore call for qualitatively different paradigms for HTSC.

Care must be taken when identifying the kinetic and potential energies [2]. Even in the original work of Chester [1], who identified the main contribution to the pairing energy in conventional superconductors, the reduction in the effective electronic potential actually corresponds to a decrease in the ionic kinetic energy. Furthermore, in the cuprates, where magnetic interactions are relevant, it is important to note that the magnetic exchange has mixed electronic kinetic and Coulombic origins. However, a simple analysis in terms of the original Ward identity shows that for an effective low-energy electronic Hamiltonian with only kinetic and Coulombic terms, the electronic kinetic energy, obtained from a trace of the product of the full single-particle Green function and the *bare* dispersion, is related to the optical experiments under the conditions described in Ref. [3].

One such model with separate kinetic and Coulombic terms is the two-dimensional (2D) Hubbard model. It was realized early in the history of HTSC that in the intermediate coupling regime, where the Coulomb interaction between electrons is of the order of the bandwidth, this model should capture the essential low-energy physics of the cuprates [5]. However, this model lacks exact solutions and approximative methods have to be applied. The foundation of the BCS theory relies upon a small parameter, the ratio of the Debye frequency to the Fermi energy ω_D/E_F. One of the complications of the purely electronic models of HTSC is the lack of such a small parameter expressible as the ratio of energy scales. Perhaps the most natural expansion parameter for these systems comes from the length scale of antiferromagnetic spin correlations. Neutron scattering experiments confirm the presence of short-ranged antiferromagnetic correlations in the doped cuprates up to length scales ξ roughly equal to the mean distance between holes, or roughly one lattice spacing in the optimally doped cuprates [6]. In the dynamical cluster approximation [7–10] (DCA) we take advantage of the short length scale of antiferromagnetic correlations to map the original lattice model onto a periodic cluster with linear size L_c embedded in a self-consistent host and use $(\xi/L_c)^2$ [8] as the small parameter. As a result, dynamical correlations up to a range $\sim L_c$ are treated accurately while the physics on longer length scales is described on a mean-field level. We solve the cluster problem using quantum Monte Carlo and obtain dynamics from the maximum entropy method [11].

We investigate the nature of the superconducting phase transition of the conventional 2D Hubbard model on a square lattice. The model is characterized by a hopping integral t between nearest neighbor sites and a Coulomb repulsion U two electrons feel when residing on the same site. As the energy scale we set $t = 0.25$ eV so that the bandwidth $W = 8t = 2$ eV. We simulate the superconducting and corresponding normal state solutions down to temperatures $T \approx 0.5T_c$ and compare their respective kinetic and potential energies. To obtain the normal state solution we suppress superconductivity by not allowing for any symmetry breaking in our representation.

To illustrate the typical BCS behavior we study the superconducting instability in the negative U, i.e., attractive Hubbard model, which for $|U| \ll W$ is expected to show BCS behavior. Because of the local nature of the attractive potential U between electrons, the superconducting order parameter has s-wave symmetry and hence single-site DCA simulations ($N_c = 1$) can capture the mean-field behavior of this transition. Figure 1 shows our $N_c = 1$ data for the negative U model for $U = -0.375W$ at doping $\delta = 0.05$. As expected, pairing is driven by a reduction of the electronic potential energy, while the kinetic energy slightly increases in the superconducting state.

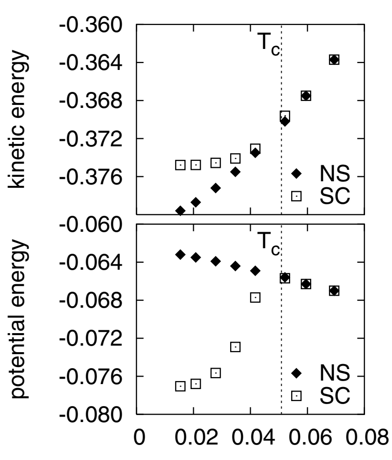

FIG. 1. Kinetic (top) and potential (bottom) energies of the normal (NS) and superconducting (SC) states in the negative U Hubbard model ($U = -0.375W$) for $N_c = 1$ as a function of temperature across the superconducting transition at $T_c \approx 0.051$ as indicated by the dashed line at 5% doping. Pairing is accompanied by a reduction of the electronic potential energy and by a slight increase of the kinetic energy.

We now turn to the actual focus of this Letter, the positive U, i.e., repulsive Hubbard model. We set the Coulomb repulsion equal to the bandwidth, $U = W$, to study the relevant, intermediate coupling regime for a description of the HTSC. We explore the dynamics on short length-scales by setting the cluster size to $N_c = 4$, the smallest cluster size which allows for a superconducting phase with d-wave order parameter. We have previously shown that this cluster size is large enough to capture the qualitative low-energy physics of the cuprate superconductors [12,13], while the solution retains some mean-field behavior: We find antiferromagnetism and pseudogap behavior at low doping and a transition to a superconducting state with d-wave symmetry at low temperatures over an extended range of finite dopings.

In this Letter, we are interested in the nature of the superconducting phase transition. We study whether pairing in the repulsive Hubbard model is driven by the existence of an attractive pairing potential as in the BCS theory and weak coupling attractive Hubbard model, or a lowering of the kinetic energy. In Fig. 2 we present the kinetic (top) and potential (bottom) energies as a function of temperature at low doping ($\delta = 0.05$) on the left panel and high doping ($\delta = 0.20$) on the right panel. The corresponding values of the critical temperatures T_c are indicated by the vertical dotted lines. For both doping levels, the kinetic energy of the superconducting state is lower than the kinetic energy of the corresponding normal state solution. This contradicts the behavior expected from BCS theory where the kinetic energy of the superconducting state is always slightly increased compared to the normal state. In addition, the potential energies of the normal and superconducting states are almost identical,

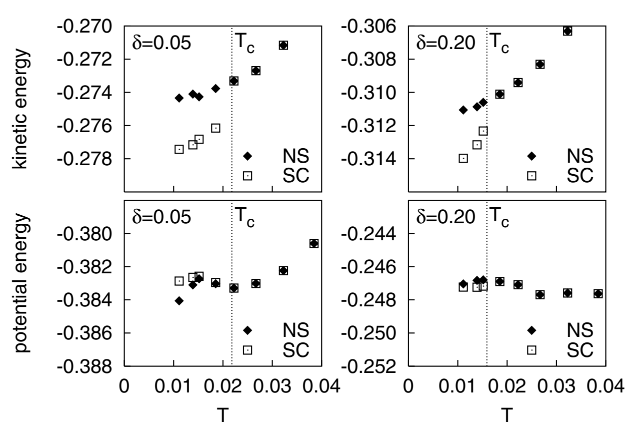

FIG. 2. Kinetic (top) and potential (bottom) energies of the repulsive Hubbard model in the normal (NS) and superconducting (SC) states as a function of temperature for low doping ($\delta = 0.05$, left) and high doping ($\delta = 0.20$, right). The vertical dotted lines represent the value of T_c. Pairing is mediated by a reduction of the kinetic energy.

indicating that pairing is not driven by the potential energy. The magnitude of the kinetic energy lowering at low doping, measured relative to the transition temperature, is roughly $(\Delta E_{\rm kin}/k_{\rm B}T_c) \approx 0.18$, in good agreement with the experimental estimate of $(\Delta E_{\rm kin}/k_{\rm B}T_c) \approx (1\,{\rm meV}/k_{\rm B}66\,{\rm K}) \approx 0.18$. At $\delta = 0.20$, the lowering of the kinetic energy is slightly less compared with $\delta = 0.05$. We conclude that superconductivity in the Hubbard model is driven by a lowering of the kinetic energy with a magnitude that decreases as doping increases.

What could be the underlying microscopic mechanism for the observed kinetic energy driven pairing in HTSC and our simulation? Because of the vicinity of the superconducting phase to antiferromagnetic ordering, it is widely believed that short-ranged antiferromagnetic spin correlations are responsible for pairing in the cuprates. This is the essential idea behind two pairing models which predict the experimentally observed lowering of the electronic kinetic energy. The first one relies on the existence of quasiparticles and is partially based on studies [14–17] of the motion of holes in an antiferromagnetic background which date back to the early work of Brinkman and Rice [18]. The motion of a single hole is inhibited because it creates a string of broken antiferromagnetic bonds. Based on this picture, it is argued that two holes can decrease their kinetic energy by traveling together, in a coherent motion, i.e., by forming Cooper pairs. Hirsch's discussion of kinetic energy driven superconductivity [19] is consistent with this picture. The second idea, due to Anderson, involves spin-charge separation within a resonating valence bond (RVB) picture [20]. Because of strong antiferromagnetic correlations, spins pair into short-ranged singlets at a temperature T^* much higher than the superconducting transition temperature T_c. This leads to a pseudogap in the electronic excitation spectrum and consequently to an increase in kinetic energy. Contrary to the quasiparticle picture, the elementary excitations of this state are spin 1/2 charge neutral Fermions called spinons, and spin 0 bosons called holons. At T_c the holons become coherent and recombine with the spinons, forming electrons which pair and render the system superconducting. Frustrated kinetic energy is then recovered [21].

The first picture relies on the existence of quasiparticles, which in the Fermi-liquid concept correspond one to one to with those of a Fermi gas and thus have charge and spin. Anderson's RVB scenario, on the other hand, is based on the concept of spin-charge separation and predicts quasifree charge excitations, the holons. To distinguish between these two models we investigate the low-energy quasiparticle and charge excitations in the Hubbard model by calculating the single-particle spectral function $A(\mathbf{k}, \omega)$ and the dynamic charge susceptibility, respectively. Our result for $A(\mathbf{k}, \omega)$ in the weakly doped system ($\delta = 0.05$) for the temperature $T = 0.022$ below the pseudogap temperature T^* and slightly above the critical temperature T_c is presented in the left panel of Fig. 3. While coherent quasiparticle peaks exist along $\Gamma \to$ M, a pseudogap, i.e., a partial suppression of low-energy spectral weight is seen near $X = (\pi, 0)$ at the Fermi energy ($\omega = 0$). Since the superconducting order parameter has a d-wave form, this is the region in k space where Cooper pairs are formed. This clearly indicates that no quasiparticles in the normal state contribute to pairing. In the right panel of Fig. 3 we show the imaginary part of the local dynamic charge susceptibility $\chi_c''(\omega)$ divided by the frequency for different temperatures. The low frequency behavior of this quantity provides insight in the low-energy charge excitations. As the temperature decreases, this quantity develops a strong peak at zero frequency, indicating the emergence of coherent charge excitations.

Since $A(\mathbf{k}, \omega)$ represents quasiparticle excitations which have both charge and spin, it follows from the simultaneous emergence of a pseudogap in $A(\mathbf{k}, \omega)$ and the development of coherent charge excitations that the low-energy spin excitations must be suppressed. And indeed, our results for the spin susceptibility at the antiferromagnetic wave vector (π, π) (not shown) display this suppression of spin excitations. Thus, at temperatures below the crossover temperature $T^\star$ spin and charge degrees of freedom behave qualitatively differently, suggesting spin and charge separation.

Figure 4 shows the behavior of the density of states $N(\omega) = 1/N\sum_{\mathbf{k}} A(\mathbf{k}, \omega)$ (left panel), charge (center panel), and spin susceptibility (right panel) at 5% doping as the temperature decreases below the superconducting transition temperature $T_c = 0.0218$. The density of states and the spin susceptibility change smoothly across the superconducting phase transition. The pseudogap in both quantities changes to a superconducting gap [22] below

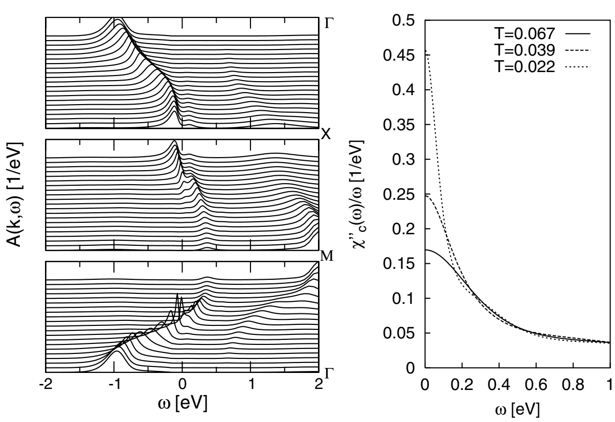

FIG. 3. The low-energy single-particle spectral function $A(\mathbf{k}, \omega)$ at temperature $T = 0.022$ along high-symmetry directions in the Brillouin zone between $\Gamma = (0, 0)$, $X = (\pi, 0)$, and $M = (\pi, \pi)$ (left) and the imaginary part of the local charge susceptibility over the frequency (right) at weak doping ($\delta = 0.05$) for different temperatures. While a pseudogap exists in $A(\mathbf{k}, \omega)$, a peak develops at zero frequency in the charge susceptibility.

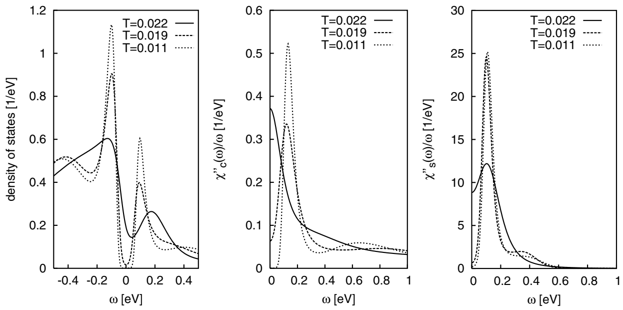

FIG. 4. The density of states (left), local dynamic charge susceptibility (center), and local dynamic spin susceptibility (right) when $\delta = 0.05$ and $T_c = 0.0218$. Note that for $T \ll T_c$ all quantities display a narrow peak delimiting the superconducting gap, indicating the formation of quasiparticles.

T_c. However, since the charge susceptibility is peaked at zero frequency even slightly above T_c, it changes abruptly upon pairing to show the same behavior as the spin susceptibility, including the superconducting gap at low frequencies. Remarkably, well below T_c all quantities display narrow peaks at $\omega \approx 0.1$ eV delimiting the superconducting gap. This clearly indicates the formation of quasiparticles below T_c.

These results may be interpreted within a spin-charge separated picture similar to that described in Anderson's RVB theory. The pairing of spins in singlets below the crossover temperature $T^\star$ results in the suppression of low-energy spin excitations and consequently in a pseudogap in the density of states. The holons, or charge excitations are quasifree as indicated by the zero-frequency peak in the charge susceptibility. Well below the transition spin and charge degrees of freedom recombine, forming electrons which pair. Frustrated kinetic energy is recovered as indicated by the reduction of the kinetic energy as the system goes superconducting. However, since spinons are not observables in our calculation, their existence cannot be directly addressed. Furthermore, since the DCA treats long-ranged correlations with a single-particle mean-field host, we can only have spin-charge separation at short time and length scales within the cluster. It is interesting to note that a weak shoulder appears in the charge susceptibility at $\omega = 0.4 \approx zJ$, where z is the coordination number and $J = 4t^2/U$ the antiferromagnetic coupling between neighboring spins. This observation might be interpreted as a remanence of residual spin-charge coupling.

Using the dynamical cluster approximation we find a kinetic energy driven instability in the 2D Hubbard model, consistent with recent optical experiments. The transition is from a state with partial spin-charge separation to a d-wave superconducting state with quasiparticle excitations.

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[1] G. Chester, Phys. Rev. **103**, 1693 (1956).
[2] M. R. Norman, M. Randeria, B. Jankó, and J. C. Campuzano, Phys. Rev. B **61**, 14 742 (2000).
[3] H. J. A. Molegraaf, C. Presura, D. van der Marel, P. H. Kes, and M. Li, Science **295**, 2239 (2002).
[4] A. F. Santander-Syro, R. P. S. M. Lobo, N. Bontemps, Z. Konstantinovic, Z. Z. Li, and H. Raffy, cond-mat/0111539.
[5] P.W. Anderson, *The Theory of Superconductivity in the High-T_c Cuprates* (Princeton University Press, Princeton, NJ, 1997).
[6] T. R. Thurston *et al.*, Phys. Rev. B **40**, 4585 (1989).
[7] M. H. Hettler, A. N. Tahvildar-Zadeh, M. Jarrell, T. Pruschke, and H. R. Krishnamurthy, Phys. Rev. B **58**, R7475 (1998).
[8] M. H. Hettler, M. Mukherjee, M. Jarrell, and H. R. Krishnamurthy, Phys. Rev. B **61**, 12739 (2000).
[9] T. Maier, M. Jarrell, T. Pruschke, and J. Keller, Eur. Phys. J. B **13**, 613 (2000).
[10] M. Jarrell and H. R. Krishnamurthy, Phys. Rev. B **63**, 125102 (2001).
[11] M. Jarrell, T. Maier, C. Huscroft, and S. Moukouri, Phys. Rev. B **64**, 195130 (2001).
[12] M. Jarrell, T. Maier, M. H. Hettler, and A. N. Tahvildarzadeh, Europhys. Lett. **56**, 563 (2001).
[13] T. Maier, M. Jarrell, T. Pruschke, and J. Keller, Phys. Rev. Lett. **85**, 1524 (2000).
[14] J. E. Hirsch, Phys. Rev. Lett. **59**, 228 (1987).
[15] J. Bonca, P. Prelovsek, and I. Sega, Phys. Rev. B **39**, 7074 (1989).
[16] E. Dagotto, J. Riera, and A. P. Young, Phys. Rev. B **42**, 2347 (1990).
[17] T. Barnes, A. E. Jacobs, M. D. Kovarik, and W. G. Macready, Phys. Rev. B **45**, 256 (1992).
[18] W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 1324 (1970).
[19] J. E. Hirsch, Science **295**, 2226 (2002).
[20] P.W. Anderson, Science **235**, 1196 (1987).
[21] G. Baskaran, Int. J. Mod. Phys. B **14**, 2117 (2000).
[22] Note that due to the finite resolution in momentum space, the DCA underestimates low-energy spectral weight in superconductors where the gap has nodes on the Fermi surface. As a result we find a fully developed gap at low temperatures instead of a density of states that vanishes linearly in frequency as expected for a d-wave superconductor.