Kinetic energy driven pairing

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Pairing occurs in conventional superconductors through a reduction of the electronic potential energy accompanied by an increase in kinetic energy, indicating that the transition is driven by a pairing potential. 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 the nature of superconductivity in a microscopic model of the cuprates, the two-dimensional Hubbard model. We find that pairing is indeed driven by the kinetic energy and that superconductivity evolves from an unconventional, spin-charge separated state, consistent with the RVB model of high-temperature superconductors.

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 reduce by forming Cooper pairs. However, recent optical experiments show that the transition in the cuprates is due to a lowering of 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, the quanta of ionic vibrations of the crystal. Since this interaction leads to a net attractive force between electrons, the system can lower its potential energy by forming pairs which have s-wave symmetry due to the local nature of the pairing interaction. These “Cooper-pairs” condense into a coherent macroscopic quantum state, insensitive to impurities and imperfections, and as a result, electricity can be conducted without resistance.

The scattering of Cooper-pairs mediated by the attractive interaction leads to a reduction of its potential energy. To take 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 kinetic energy which is overcompensated by the lowering of 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. In the normal state of the weakly doped cuprates no quasiparticles are found, undermining the very foundation of BCS theory. It is widely believed that phonons cannot be responsible for pairing at temperatures as high as 160K. Consistently, the pairs have d-wave symmetry, instead of s-wave symmetry. Most significantly, new optical experiments call for qualitatively different paradigms for HTSC. These experiments have shown 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.

Early in the history of HTSC it was realized that the two-dimensional (2D) Hubbard model in the intermediate coupling regime, where the Coulomb interaction between electrons is of the order of the bandwidth, should capture the essential low-energy physics of the cuprates. However, these models lack 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 $\omega_D/E_F$. One of the complications of the purely electronic models of HTSC is the lack of such a small parameter since the Coulomb repulsion between electrons is roughly equal to their bandwidth. Perhaps the most natural expansion parameter for these systems is 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 roughly equal to the mean distance between holes, or roughly one lattice spacing in the optimally doped cuprates with the highest transition temperature $T_c$. In the dynamical cluster approximation (DCA) we take advantage of the short length-scale of antiferromagnetic correlations and use it as a small parameter. The DCA reduces the complexity of the problem by coarse-graining the k-space on a scale $2\pi/L_c$. As a result, dynamical correlations up to a range $\sim L_c/2$ are treated accurately while the physics on longer length scales is described on a mean-field level. The original lattice problem is mapped onto a periodic cluster of size $N_c = L_c^D$ in $D$ dimensions embedded in a host which has to be determined self-consistently. We solve the cluster problem using quantum Monte Carlo and obtain dynamics from the maximum entropy method.

We present results of DCA calculations for the conventional 2D Hubbard model describing the dynamics of electrons 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 $t = 0.25eV$ so that the band-width $W = 8t = 2eV$, and study the intermediate coupling regime $U = W$. We study 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. This cluster size is large enough to capture the qualitative low-energy physics of the cuprate superconductors \([10, 11]\), while the solution retains some mean-field behavior.

These results are summarized in the temperature-doping ($T$-$\delta$) phase diagram shown in Fig. 1. At low doping $\delta$ the system is an antiferromagnetic insulator below the Neél-temperature $T_N$. At finite doping $\delta \leq 0.3$ we find an instability at the critical temperature $T_c$ to a superconducting state with a $d$-wave order parameter. In the normal state low-energy spin excitations become suppressed below the crossover temperature $T^*$. Simultaneously the electronic excitation spectrum represented by the density of states displays a pseudogap, i.e. a partial suppression of low-energy spectral weight (see left panel of Fig. 1).

In this Letter, we investigate the nature of this transition from the normal to the superconducting state and in particular study whether pairing in the Hubbard model is driven by the existence of an attractive pairing potential as in the BCS theory of superconductivity, or a lowering of the kinetic energy. To this end we simulate the superconducting and corresponding normal state solutions of the Hubbard model 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.

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. As expected, below $T_c$ the energies of the normal and superconducting state start to differ. 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, 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 $\frac{\Delta E_{kin}}{k_B T_c} \approx 0.15$, in good agreement with the experimental estimate of $\frac{\Delta E_{kin}}{k_B T_c} \approx 1meV = 0.15$. At $\delta = 0.20$, the lowering of the kinetic energy is slightly less compared with $\delta = 0.05$. Thus 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? Due to 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 in kinetic energy. The first one relies on the existence of quasiparticles and is partially based on studies \[12, 13, 14, 15\] of the motion of holes in an antiferromagnetic background which date back to the early work of Brinkman and Rice \[14\]. 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 \[17\] is consistent with this picture. The second idea, due to Anderson, involves spin-charge separation within a resonating valence bond (RVB) picture \[18\]. Due to 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 \(T\), the holons become coherent and recombine with the spinons, forming electrons which pair and render the system superconducting. Frustrated kinetic energy is then recovered \[19\].

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 quasi-free 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 density of states near the Fermi level \(\omega = 0\) for different \(\delta = 0.05\) for different temperatures above the critical temperature \(T_c\) is presented in the left panel of Fig. 3. As the temperature decreases below the crossover temperature \(T^*\), a pseudogap develops in the density of states near the Fermi energy \(\omega = 0\). This partial suppression of low-energy spectral weight clearly indicates that no quasiparticles are present in the normal state close to the superconducting transition. In the right panel of Fig. 3 we show the imaginary part of the local dynamic charge-susceptibility \(\chi''\) 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 the density of states represents quasiparticle excitations which have both charge and spin, it follows from the simultaneous emergence of a pseudogap in the density of states 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 \((\pi, \pi)\) (not shown) display this suppression of spin-excitations. Thus, at temperatures below the crossover temperature \(T^*\) spin and charge degrees of freedom behave qualitatively different, indicating spin and charge separation. 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. This observation might be interpreted as a remanence of a residual spin-charge coupling.

Fig. 3 shows the behavior of the density of states (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 \(20\) below \(T_c\). 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 \(\omega \approx 0.1eV\) delimiting the superconducting gap. This clearly indicates the formation of quasiparticles below \(T_c\).

These results can thus be interpreted within a spin-charge separated picture as described in Anderson’s RVB theory. The pairing of spins in singlets below the
crossover temperature $T^*$ 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 free 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.

Using the dynamical cluster approximation we find a kinetic energy driven instability in the 2D Hubbard model from an RVB state to a $d$-wave superconducting state consistent with recent optical experiments.

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[20] 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.
FIG. 4: The density of states (right), local dynamic charge susceptibility (center), and the local dynamic spin susceptibility (right) when $\delta = 0.05$, $T_c = 0.0218$. Note that for $T \ll T_c$, all quantities display a narrow peak delimiting the superconducting gap, indicating the formation of quasiparticles.