Potential-energy-driven (BCS) to kinetic-energy-driven (BEC) pairing in the two-dimensional attractive Hubbard model: Cellular dynamical mean-field theory

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The BCS-BEC crossover within the two-dimensional attractive Hubbard model is studied by using the Cellular Dynamical Mean-Field Theory, both in the normal and superconducting ground states. Short-range spatial correlations incorporated in this theory remove the normal-state quasiparticle peak and the first-order transition found in the Dynamical Mean-Field Theory, rendering the normal state crossover smooth. For U smaller than the bandwidth, pairing is driven by the potential energy, while in the opposite case it is driven by the kinetic energy, resembling a recent optical conductivity experiment in cuprates. Phase coherence leads to the appearance of a collective Bogoliubov mode in the density-density correlation function and to the sharpening of the spectral function.

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The problem of the crossover between the BCS and the Bose-Einstein condensation (BEC) has been of great interest in the context of the pseudogap observed in underdoped cuprates.[1] The recent discovery of the BCS-BEC crossover in ultracold fermionic atoms trapped in optical lattices[2] has renewed our interest in this issue. Does the condensation of loosely bound Cooper pairs evolve smoothly into the BEC of tightly bound composite bosons as the attraction between fermions is increased gradually? This question was first addressed by Leggett,[3] who proposed that these two pictures are limiting cases of a more general theory in which both the fermionic nature of individual particles and the bosonic nature of pairs must be considered on an equal footing. By using a T-matrix approximation in the intermediate coupling regime, Nozières and Schmitt-Rink[4] extended Leggett's analysis to a lattice and to finite temperature to find a smooth connection between the two limits. Since then, various other approximate schemes have been used to understand the pseudogap phenomena as well as the BCS-BEC crossover. For example, Quantum Monte Carlo (QMC) simulations[5–7] of the two- and three-dimensional attractive Hubbard model found a breakdown of Fermi liquid theory in the normal state, accompanied by a pseudogap and a spin gap.

The first Dynamical Mean-Field Theory (DMFT)[8] study of the BCS-BEC crossover at arbitrary attractive interactions was carried out by Keller *et al.*[9] The authors calculated the transition temperature for superconductivity, which smoothly interpolates from the BCS behavior at weak coupling to the t^2/U behavior at strong coupling. However, the double occupancy, the spin susceptibility, and the quasiparticle weight show, in the $T \rightarrow 0$ limit of their *normal state* solution, a discontinuity near $U \sim 1.5W$, with W the bandwidth. Capone *et al.*[10] studied the first-order transition in detail by using exact diagonalization as the impurity solver for DMFT and later extended their work to finite temperature.[11] The discontinuity found in the normal state of DMFT may suggest a *radically* different mechanism for superconductivity at weak and strong coupling, but that is problematic in the context of the expected smooth BCS-BEC crossover (in the superconducting state). Nevertheless, in a recent optical conductivity experiment in the cuprates, Deutscher *et al.*[12] found that near optimal doping there is a reversal of the sign of the kinetic energy difference between the superconducting (SC) and normal (NR) states. Although the mechanism for superconductivity in the cuprates is still under debate, this intriguing experiment calls for an explanation also in the context of the BCS-BEC crossover, as the authors noted.

In the BCS limit, it is well established that superconductivity is potential-energy driven since the broadening of the Fermi surface caused by superconductivity leads to an increase in kinetic energy in the superconducting state. At strong coupling, in the BEC limit, one may expect that superconductivity is kinetic-energy driven based on two different arguments: (a) The gain in potential energy occurs at a high temperature, where the bosons form. At low temperature, to leading order in a low density expansion,[13] the bosons condense for the same reason as free bosons, because of the gain in kinetic energy. Hence, comparing with a normal state where the bosons are formed, the superconductivity occurs because of a gain in kinetic energy. (b) One can map the attractive Hubbard model to the half-filled repulsive model in the presence of a magnetic field. The antiferromagnetic order that appears close to half-filling in this model is analogous to superconductivity and at strong coupling it occurs because having neighbors that are ordered leads to a gain in exchange energy.[14] One can check that in the mapping of the Hubbard model to the Heisenberg or t-J model, the exchange energy corresponds to minus twice the potential energy of the original Hubbard model.[15] These physical arguments do not tell us whether the change in pairing mechanism occurs in a continuous or discontinuous manner, at what coupling they occur, or what is the order of magnitude of the condensation energy. The explicit calculations presented in the present paper thus answer both qualitative and quantitative questions.

First we emphasize our main results: (1) Including short-range spatial correlations explicitly removes the first-order transition found in DMFT, rendering the crossover in the NR

state also smooth, without a discontinuity, just as in the SC state. (2) Near U equal to the bandwidth of $8t$, a change in the pairing mechanism occurs. For $U<8t$ the condensation energy is lowered by the potential energy while for $U>8t$ it is lowered by the kinetic energy, resembling a recent optical conductivity experiment.[12] (3) The phase coherence manifests itself most dramatically by the appearance of a collective Bogoliubov mode in the density-density correlation function and by the sharpening of the spectral function compared with the normal state.

Using Cellular Dynamical Mean-Field Theory (CDMFT),[16] we study the crossover between weak and strong-coupling in the two-dimensional attractive Hubbard model,[17]

$$H = \sum_{\langle ij\rangle,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} - U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} c_{i\sigma}^{\dagger} c_{i\sigma}, \qquad (1)$$

where $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) are creation (annihilation) operators for electrons of spin σ, $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$ is the density of σ spin electrons, t_{ij} is the hopping amplitude equal to $-t$ for nearest neighbors only, $-U$ is the on-site attractive interaction with $U>0$ and μ is the chemical potential controlling the electron density. The CDMFT method is a natural generalization of the single site DMFT[8] that incorporates short-range spatial correlations. In the CDMFT construction[16,18] the infinite lattice is tiled with identical clusters of size N_c, and the degrees of freedom in the cluster are treated exactly while the remaining ones are replaced by a bath of noninteracting electrons that is determined self-consistently. Since the CDMFT method treats short-range spatial correlations explicitly, it is able to describe features caused by the finite dimensionality or finite coordination number, which are missed in the single site DMFT.

To solve the quantum cluster embedded in an effective SC medium, we consider a cluster-bath Hamiltonian of the form[19,20]

$$H = \sum_{\langle\mu\nu\rangle,\sigma} t_{\mu\nu} c_{\mu\sigma}^{\dagger} c_{\nu\sigma} - U \sum_{\mu} n_{\mu\uparrow} n_{\mu\downarrow} + \sum_{m,\sigma,\alpha} \varepsilon_{m\sigma}^{\alpha} a_{m\sigma}^{\dagger\alpha} a_{m\sigma}^{\alpha} + \sum_{m,\mu,\sigma,\alpha} V_{m\mu\sigma}^{\alpha} (a_{m\sigma}^{\dagger\alpha} c_{\mu\sigma} + \text{H.c.}) + \sum_{m,\alpha} \Delta (a_{m\uparrow}^{\alpha} a_{m\downarrow}^{\alpha} + \text{H.c.}). \qquad (2)$$

Here the indices $\mu,\nu=1,\ldots,N_c$ label sites within the cluster, and $c_{\mu\sigma}$ and $a_{m\sigma}^{\alpha}$ annihilate electrons on the cluster and the bath, respectively. In the present study we used $N_c=4$ sites for the cluster (minimum number of sites reflecting the full square lattice symmetry) and $N_b=8$ sites for the bath with $m=1,\ldots,4,\alpha=1,2$. $t_{\mu\nu}$ is the hopping matrix within the cluster and, using symmetry, $\varepsilon_{m\sigma}^{\alpha}=\varepsilon^{\alpha}$ is the bath energy and $V_{m\mu\sigma}^{\alpha}=V^{\alpha}\delta_{m,\mu}$ is the bath-cluster hybridization matrix. Δ represents the amplitude of s-wave SC correlations in the bath. To deal with superconductivity, the Nambu spinor representation is used for the cluster operators,

$$\Psi^{\dagger} = (c_{1\uparrow}^{\dagger}, c_{2\uparrow}^{\dagger}, c_{3\uparrow}^{\dagger}, c_{4\uparrow}^{\dagger}, c_{1\downarrow}, c_{2\downarrow}, c_{3\downarrow}, c_{4\downarrow}),$$

while the Weiss field, the cluster Green's function, and self-energy constructed from these operators are 8×8 matrices. The exact diagonalization method[21] is used to solve the cluster-bath Hamiltonian Eq. (2) at zero temperature, which has the advantages of computing dynamical quantities directly in real frequency and of treating the large U regime without difficulty. All the results presented here are obtained at quarter filling ($n=1/2$) far from the particle-hole symmetric case where charge-density-wave and pairing instabilities coexist. Qualitatively similar results were found at other densities.

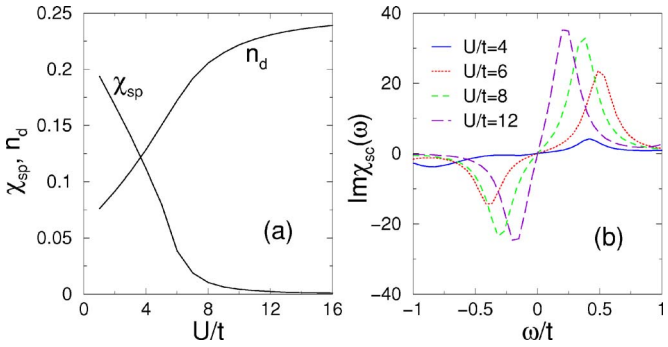

FIG. 1. (Color online) (a) Uniform static cluster spin susceptibility χ_{sp} and double occupancy $n_d=<n_{i\uparrow}n_{i\downarrow}>$. (b) Imaginary part of the s-wave cluster pair correlation function with total momentum equal to zero $\chi_{sc}(\omega)$. The above quantities are calculated in the NR ground state at quarter filling ($n=1/2$).

Figure 1(a) presents the evolution with U of the uniform static cluster spin susceptibility χ_{sp} and of the double occupancy n_d in the NR state obtained by forcing SC order to vanish. In the case of the attractive Hubbard model, χ_{sp} and n_d describe how many fermions turn into local singlet pairs due to attraction. In the limit of $U\to\infty$, $\chi_{sp}\to0$ and $n_d\to n/2$, while in the opposite limit, $\chi_{sp}\to2N(0)$ and $n_d\to(n/2)^2$. Here $N(0)$ is the (noninteracting) density of states per spin. From weak to strong coupling, these thermodynamic quantities are continuous in CDMFT, in stark contrast to those of the single site DMFT (see Fig. 2 and Fig. 3 in Ref. 9). Near $U/t=8$, both χ_{sp} and n_d start to saturate, indicating that tightly bound bosonic pairs[17] begin to dominate the physics.

Figure 2 shows additional evidence of the absence of a first order transition when short-range correlations are treated explicitly. Unlike in DMFT, where the spectral function $A(\mathbf{k},\omega)$ has a peak at $\omega=0$ that disappears at a critical coupling $U_c/t\simeq12$ (Ref. 22) to lead to an insulator, in CDMFT $A(\mathbf{k},\omega)$ is a minimum at $\omega=0$ already at $U/t=6$, and we claim that the apparent absence of a gap at $U/t=4$ (the first panel) is an artifact of the finite size of the cluster used. In the case of weak coupling, short-range correlations available in a cluster of size $N_c=4$ are not long enough to lead to a gap, as was found in the repulsive Hubbard model.[23] When a large 64×64 lattice is used to capture long-range correlation effects within the Two-Particle Self-Consistent (TPSC) theory[24] (dashed curve) valid at weak coupling, a gaplike feature does exist, even at a finite temperature of $T/t=1/8$. QMC calculations on a 16×16 lattice[7] show the same result. Hence, there is enough evidence that as soon as finite-range spatial correlations are included explicitly, the first order transition from a Fermi liquid to a non-Fermi liquid state found in the NR state solution of the DMFT equations dis-

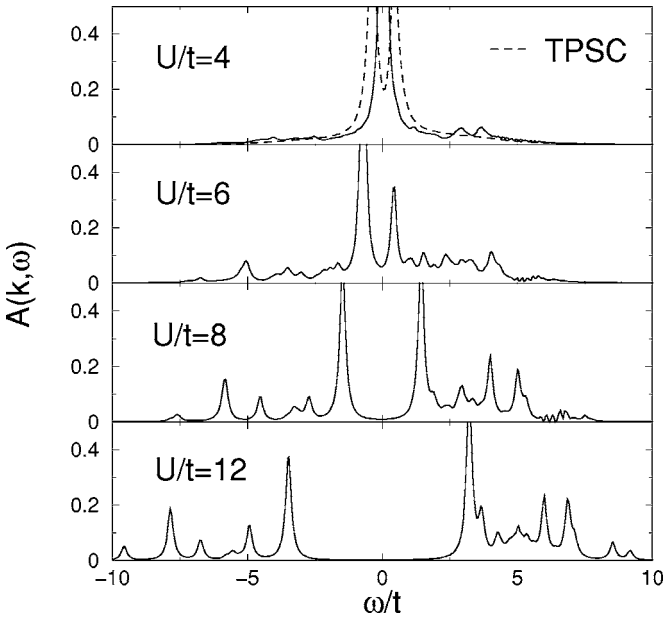

FIG. 2. Single particle spectral function $A(\mathbf{k},\omega)$ at $\mathbf{k}=(3/8\pi,3/8\pi)$ near the Fermi surface calculated in the NR ground state with a broadening parameter of $0.125t$. The dashed curve in the first panel is computed from the TPSC at finite temperature of $\beta=t/T=8$ on a 64×64 cluster.

appears immediately,[25] making the NR state crossover smooth,[26] just as in the SC state. Physically, the reason why DMFT leads to a first-order transition is because residual hopping between preformed pairs is of order $t^2/U\times1/d$ with d the dimension, hence they have vanishing kinetic energy contribution in large dimension and they localize. Within CDMFT, boson hopping is restored (within the clusters). With increasing U, $A(\mathbf{k},\omega)$ has a large incoherent spectrum at high frequencies together with a sharp peak near the gap edge. A close inspection shows a continuous evolution of high energy peaks for $U/t\geqslant6$.

The smooth crossover can also be seen by considering Fig. 1(b), which shows the imaginary part of the s-wave cluster pair correlation function computed in the NR state for several couplings. With increasing U beyond $6t$, the peak intensity increases, while the peak position decreases, scaling as J. This is analogous to the t^2/U scaling of the peak position in the spin-spin correlation function at $\mathbf{q}=(\pi,\pi)$ in the half-filled Hubbard model.[27] The gradual change of the pair correlation function from weak to strong coupling is consistent with the smooth crossover of $A(\mathbf{k},\omega)$ as a function of U.

Next, we study the BCS-BEC crossover in the SC state and its consequences. Figure 3(a) shows the kinetic E_K, potential E_U, and total E_T energies computed in the SC and NR ground states, denoted as the solid and dashed curves, respectively. Generally the energy differences are tiny (only about 1%–2%), which implies that the two ground states are energetically very close. At weak coupling one finds, as in the BCS theory,[28] that while kinetic energy is increased in the SC state by the broadening of the Fermi surface, the decrease in the potential energy overcompensates it. At strong coupling, however, the roles are interchanged. On a lattice, phase coherence involves breaking up of more local

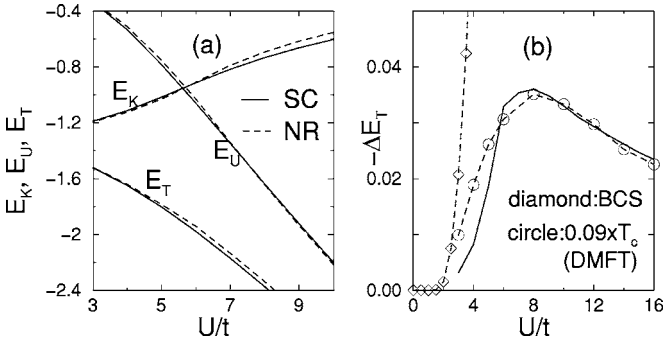

FIG. 3. (a) Kinetic E_K, potential E_U, and total E_T energies computed in the SC and NR ground states denoted as the solid and dashed curves, respectively. (b) The total energy difference between the SC and NR states ΔE_T. The condensation energy obtained from the BCS theory is shown as diamonds. The circles represent T_c obtained by Keller *et al.* (Ref. 9) within DMFT but multiplied by 0.09.

pairs by virtual hopping (increase in the potential energy) to enhance their mobility further (a decrease in the kinetic energy). The full inversion of the roles occurs near $U/t=8$, but the decrease in kinetic energy happens somewhat earlier ($U/t=6$) in our study. Although the mechanism for high temperature superconductivity is debated and the observed gap symmetry (d wave) is different from the s wave predicted in the attractive Hubbard model, the current result resembles a recent optical conductivity experiment in the cuprates,[12] where ΔE_K crosses over from a BCS behavior ($\Delta E_K>0$) to an unconventional behavior ($\Delta E_K<0$) as the doping decreases. In both the SC and the NR states, the kinetic energy scales as t^2/U. The difference in the total energy ΔE_T is plotted in Fig. 3(b) as a solid curve. The condensation energy scales with the T_c found by Keller *et al.*[9] in DMFT (circles), namely it reaches a maximum near $U/t=8$ and decreases as t^2/U beyond it. At $U/t=4$ it is already far smaller than that in the BCS theory. Despite the identical t^2/U scaling of ΔE_T in our result and of T_c in DMFT at strong coupling, they differ by a factor of 10 approximately. This is an upper bound since one expects the mean-field-like DMFT estimate for T_c to be high because of the neglect of spatial fluctuations.

As was shown previously, phase coherence does not lead to a large gain in energy. The difference between the NR and SC states should manifest itself most dramatically in correlation functions. We computed the uniform charge-charge correlation function in the cluster in both states, as shown in Fig. 4(a). With increasing U the mode energy decreases, in sharp contrast with the NR state spectrum shown in the inset. For $U/t\geqslant6$ in the SC state, the charge excitation forms a sharp resonance much below twice the gap, while in the NR state (inset) the weight moves away from $\omega=0$ with weight around $\omega=U$ (not shown) that corresponds to breaking a pair. In fact, it is a collective Bogoliubov mode[29] that is separated from the continuum that comes from the breaking of Cooper pairs at higher energy (not shown). Because a local pair becomes well defined only at strong coupling, the difference between the two states is most pronounced for $U/t=8$ and beyond. The difference between the two states also appears in the local density of state $N(\omega)$, but is more subtle, as

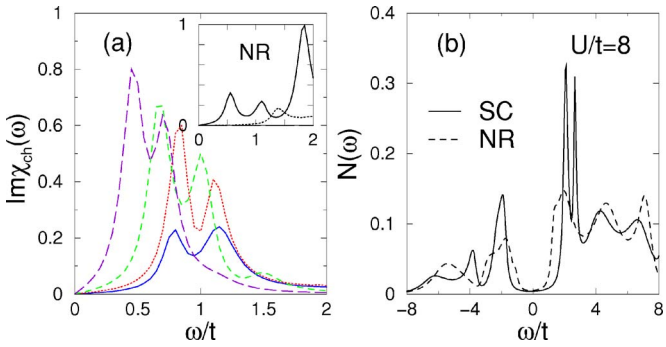

FIG. 4. (Color online) (a) An imaginary part of the collective cluster charge excitations $\chi_{ch}(\omega)$ at $\mathbf{q}=0$ in the SC and NR (inset) ground states. The solid, dotted, dashed, and long-dashed curves correspond to $U/t=$ 4, 6, 8, and 12, respectively. $\chi_{ch}(\omega)$ for $U/t=8$ and 12 in the inset are invisibly small on this scale. (b) Density of states $N(\omega)$ computed in the SC (solid) and NR (dashed) states at $U/t=8$. A broadening parameter of $0.125t$ is used in (a) and (b).

shown in Fig. 4(b). Although a pairing gap without phase coherence already exists in the NR state, the condensation depletes the remnant spectrum from the gap and builds a sharp spectrum at the gap edge.

Note that in our approach the phase fluctuations are short range. Hence, long-wavelength fluctuations do not appear necessary to lead to kinetic-energy driven pairing. Also, CDMFT allows one to go beyond the Eliashberg theory. The latter is a "strong coupling" theory in a different sense than that used in the present paper. It cannot treat the case where U is of the order of the bandwidth or larger, i.e., the case where the normal state consists of bound fermions. In the present study we focus on a 2×2 cluster with 8 bath sites since the next smallest cluster size that corresponds to 0.5 filling would need unreasonable computer resources. Nevertheless low (but finite) temperature CDMFT+QMC calculations[30] lead us to believe in the robustness of our results, except at the weakest coupling.

The increasing fractional deviation of the DMFT[31] and the CDMFT order parameter and the energy gap from their corresponding BCS values with decreasing U may be caused not only by the absence of quantum fluctuations in the BCS theory, but also by the fact that clusters (in DMFT and CDMFT) are smaller than the spatial extent of the Cooper pairs in that limit.

Although short-range spatial correlations incorporated in this theory remove the first-order transition found in the NR state of DMFT, a large frustration may lead back to a first-order transition, even in CDMFT, as was found in the half-filled repulsive Hubbard model. For that model, we found for $t'/t=-0.717$ ($t'/t=1$ in the BEDT model) that a first-order transition does occur at U close to the bandwidth.[27] In the attractive Hubbard model, frustration could come from magnetic field, for example.

To summarize, we have studied the BCS-BEC crossover within the two-dimensional attractive Hubbard model by using the Cellular Dynamical Mean-Field Theory (CDMFT), both in the normal and superconducting ground states. The explicit treatment of short-range spatial correlations in this theory removes a first-order transition found in DMFT, making the normal state crossover smooth without a discontinuity. For U smaller than the bandwidth, pairing is driven by the potential energy, while in the opposite case it is driven by the kinetic energy, resembling a recent optical conductivity experiment in the cuprates. The condensation energy has a maximum at U equal to the bandwidth and scales as t^2/U at strong coupling. Phase coherence leads to the appearance of a collective Bogoliubov mode in the density-density correlation function and to the sharpening of the gap already present in the normal state spectral function.

Note added in proof. Recently, we became aware of DMFT results by Toschi, Capone, and Castellani,[32] which also showed potential-energy to kinetic-energy-driven pairing with increasing U in the single site DMFT.

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