Potential-energy (BCS) to kinetic-energy (BEC)-driven pairing in the attractive Hubbard model

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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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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 pairing mechanism occurs. For $U \leq 8t$ 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]

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

(1)

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) are creation (annihilation) operators for electrons of spin $\sigma$, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the density of $\sigma$ 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 $\mu$ 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 non-interacting electrons that is determined self-consistently. Since the CDMFT method treats short-range spatial correlations explicitly, it is able to describe features caused by 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]

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

$$+ \sum_{m, \alpha} \Delta (a_{m \uparrow}^\dagger a_{m \downarrow}^\dagger + H.c.).$$

(2)

Here the indices $\mu, \nu = 1, \cdots, N_c$ label sites within the cluster, and $c_{\mu \sigma}$ and $a_{m \sigma}$ 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 $m = 1, \cdots, 4$. $\alpha = 1, 2, 3, 4$. $t_{\mu \nu}$ is the hopping matrix within the cluster and, using symmetry, $\varepsilon_{m \sigma} = \varepsilon^\alpha$ is the bath energy and $V_{m \mu \sigma \alpha} = V_{\alpha \delta_{m, \mu}}$ is the bath-cluster hybridization matrix. $\Delta$ 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

$$\Psi^\dagger = (c_1^\dagger, c_2^\dagger, c_3^\dagger, c_4^\dagger, c_1, c_2, c_3, c_4),$$

while the Weiss field, the cluster Green’s function and self-energy matrices constructed from these operators are 8x8 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(a) presents the evolution with $U$ of the uniform static cluster spin susceptibility $\chi_{sp}$ and double occupancy $n_d = \langle n_{i\uparrow} n_{i\downarrow} \rangle$. (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 $(n = 1/2)$.
a critical coupling $U_c/t \approx 12$ \cite{22} to lead to an insulator, in CDMFT $A(\vec{k}, \omega)$ 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 \cite{22}. When a large $64 \times 64$ lattice is used to capture long-range correlation effects within the Two-Particle Self-Consistent (TPSC) theory \cite{TPSC} (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 $16 \times 16$ lattice \cite{QMC} 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 disappears immediately \cite{23}, making the NR state crossover smooth \cite{24}, 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 $t^2/U \times 1/d$ 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 $U$, $A(\vec{k}, \omega)$ 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 $U/t \geq 6$.

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 6 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 $\vec{q} = (\pi, \pi)$ in the half-filled Hubbard model \cite{27}. The gradual change of the pair correlation function from weak to strong coupling is consistent with the smooth crossover of $A(\vec{k}, \omega)$ as a function of $U$.

Next we study the BCS-BEC crossover in the SC state and its consequences. Fig. 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 \cite{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 pairs by virtual hopping (increase in the potential energy) to enhance their mobility further (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 \cite{12} where $\Delta E_K$ 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 $\Delta E_T$ is plotted in Fig. 3(b) as a solid curve. The condensation energy scales with the $T_c$ found by Keller et al. \cite{9} within DMFT.

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

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) Total energy difference between the SC and NR states $\Delta E_T$. The condensation energy obtained from the BCS theory is shown as diamonds. The circles represent $T_c$ obtained by Keller et al. \cite{9} within DMFT but multiplied by 0.09.
expects the mean-field like DMFT estimate for $T_c$ ready far smaller than that in the BCS theory. Despite states. The solid, dotted, dashed and long-dashed curves co r-

FIG. 4: (a) Imaginary part of the collective cluster charge excitations $\chi_{ch}(\omega)$ at $q = 0$ 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 visibly 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 0.125$t$ is used in (a) and (b).

(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 $\Delta E_T$ in our result and of $T_c$ in DMFT at strong coupling, they differ by a factor of 10 approximatively. This is a 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 above, 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 $U/t \geq 6$ 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 which 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 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 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 order the bandwidth or larger, i.e. the case where the normal state consists of bound fermions. The present study focuses on a $2 \times 2$ 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 lead us to believe in the robustness of our results except at the weakest coupling.

The increasing fractional deviation of the DMFT 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, 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. 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. 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, which also showed potential-energy to kinetic-energy-driven pairing with increasing $U$ in the single site DMFT.

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