First-Order Pairing Transition and Single-Particle Spectral Function in the Attractive Hubbard Model

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A dynamical mean-field theory analysis of the attractive Hubbard model in the normal phase is carried out upon restricting to solutions where superconducting order is not allowed. A clear first-order pairing transition as a function of the coupling takes place at all the electron densities out of half filling between a Fermi liquid, stable for $U < U_c$, and an insulating bound pairs phase for $U > U_c$, and it is accompanied by phase separation. The spectral function in the metallic phase is constituted by a low-energy structure around the Fermi level, which disappears discontinuously at $U = U_c$, and two high-energy features (Hubbard bands), which persist in the insulating phase.

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The experimental finding that the (zero-temperature) coherence length of cuprate superconductors is much smaller than for conventional superconductors has suggested that these compounds lie in an intermediate coupling regime, between the weak-coupling and the strong-coupling limits [1,2]. Moreover, the recent finding from angular resolved photoemission of the existence of a (pseudo)gap in the single-particle spectrum well above the superconducting critical temperature, i.e., in the normal phase, has been usually interpreted in terms of preformed Cooper pairs with no phase coherence. This gave emphasis to the relevant theoretical issues related to the description of the superconducting phase in the crossover regime between the standard BCS and the Bose-Einstein (BE) condensation together with the description of the normal state, where preformed pairs or dynamical superconducting fluctuations give rise to the pseudogap phenomenology. Regarding the pseudogap regime, various perturbative schemes have been adopted, without a firm unambiguous understanding of the electron pairing in the normal state [3].

Much attention has been devoted to the attractive Hubbard model as an almost ideal framework, where the pairing between the electrons can be described in all the different coupling regimes, without complications due to other physical effects. The Hubbard Hamiltonian reads

$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} - U \sum_i \left(n_{i\uparrow} - \frac{1}{2} \right) \left(n_{i\downarrow} - \frac{1}{2} \right), \tag{1}$$

where $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) creates (destroys) an electron with spin σ on the site i and $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{\sigma}$ is the number operator; t is the hopping amplitude and U is the Hubbard on-site attraction (we take $U > 0$, with an explicit minus sign in the Hamiltonian). Notice that, with this notation, the Hamiltonian is explicitly particle-hole symmetric, so that $\mu = 0$ corresponds to $n = 1$ (half filling). Despite its simplicity, an exact solution is still lacking for $d > 1$, and most of the known results are limited to weak ($U \ll t$) or strong ($U \gg t$) coupling, where the BCS and the BE approaches, respectively, are accurate descriptions. For $d > 2$, the ground state of the model (1) is superconducting for all values of U and all densities. At half filling the superconducting and the charge-density-wave order parameters mix, due to the enlarged symmetry group.

The possible formation of incoherent Cooper pairs in the pseudogap phase of the cuprates stimulated us to disregard the relatively well understood superconducting phase of the Hubbard model, by constraining ourselves to solutions without superconducting order. We rather focus on the physics of incoherent pairing by investigating the *normal phase* within the dynamical mean field theory (DMFT) [4,5]. The DMFT is a nonperturbative approach that neglects the spatial correlations, but fully retains the local quantum dynamics, and becomes exact in the limit of infinite dimensions. Because of the local nature of the interaction in the attractive Hubbard model, we expect that the physics of local pairing is well described (particularly in the BCS-BE crossover regime).

The existence of a *pairing transition* for the normal phase at quarter filling ($n = 0.5$) has been reported in Ref. [6], where the DMFT of the model has been performed by means of *finite temperature* quantum Monte Carlo (QMC) calculations. Such a transition occurs between a Fermi-liquid metallic phase, and a non-Fermi-liquid phase constituted by bound electron pairs with no phase coherence. In the same paper it was also reported a finite value of the quasiparticle weight $Z = [1 - \partial \Sigma(\omega)/\partial \omega]^{-1}$ for all values of U, even at the pairing transition and in the pairing phase. The relationship between this finite value of Z and the spectral properties, as well as the density dependence of the pairing transition, are still open questions that we address in this paper. We consider the Hubbard model at zero temperature on an infinite coordination Bethe lattice of bandwidth W, using the exact diagonalization to solve the impurity model [7]. This method requires a truncation of

the conduction bath to a small given number of orbitals $n_s - 1$, and allows us to compute, directly at $T = 0$, Z and the density of states (DOS) $\rho(\omega) = -1/\pi \, \mathrm{Im}G(\omega)$. A first characterization of the pairing transition may be given by noting that, on a bipartite lattice, a particle-hole transformation on the down spins $c_{i\downarrow} \rightarrow (-1)^i c_{i\downarrow}^\dagger$, leaving the up spins unchanged, maps the attractive model with a finite density n onto a half-filled repulsive model with a finite magnetization $m = n - 1$. The chemical potential becomes, accordingly, a magnetic field $h = \mu$. In the $n = 1$ case (half filling) the two models are completely equivalent. This mapping proves useful, since many known results for the repulsive model and for the Mott-Hubbard transition can be used to gain insight into the attractive model. In light of this mapping, the pairing transition may be viewed as the natural counterpart of the Mott-Hubbard transition in the presence of an external magnetic field. Within this analogy, the normal state results that we present can be regarded as representative of the physics of the attractive Hubbard model at $T > T_c$, and eventually even provide the actual low temperature behavior, if some mechanism frustrating superconductivity is effective, just like the paramagnetic solutions of the repulsive model become relevant if frustration prevents antiferromagnetic ordering.

The evolution of Z as a function of U for $n = 1$, $n = 0.5$, and $n = 0.25$ is shown in Fig. 1. The results reported here are given by a linear extrapolation in $1/n_s$ using $n_s = 8, 10, 12$. In the half-filled case, the paring state (that here coincides with the Mott insulating state) has always $Z = 0$, and Z vanishes continuously at the transition point $U/W = U_{c2}/W \simeq 1.49$, as reported in many previous studies [4,8]. The numerical value agrees very well with, e.g., the recent numerical renormalization group results of Ref. [9]. Away from half filling, the metallic solution exists for all values of $U < U_{c2}(n) < U_{c2}(n = 1)$. In this phase Z is a decreasing function of U, but it stays finite for all couplings. In particular, the disappearance of the metallic solution at U_{c2} is not associated to a vanishing Z (see inset of Fig. 1). The pairing phase solution exists in turn for $U > U_{c1}$, with $U_{c1}(n) < U_{c2}(n)$, and it also has always a finite Z. In the pairing phase Z is an increasing function, converging to the atomic limit value for large U. In the interval between $U_{c1}(n)$ and $U_{c2}(n)$, the metallic and pairing solutions coexist. For the half-filled model it is known that the metallic solution is always energetically favored in the whole coexistence range, and that the two solutions become identical at U_{c2}, where the *second-order* pairing transition occurs [10]. Away from half filling, the actual *first-order* transition occurs for an intermediate coupling U_c ($U_{c1} < U_c < U_{c2}$), when the energy of the pairing state becomes lower than the metallic one. The value of U_c (marked by vertical arrows in Fig. 1) is maximum in the special half-filling case and decreases with increasing doping. In the extreme dilute limit $n \rightarrow 0$, the pairing transition coincides with the binding of two electrons, and it occurs for $U_{c0} = 0.56W$. We emphasize that,

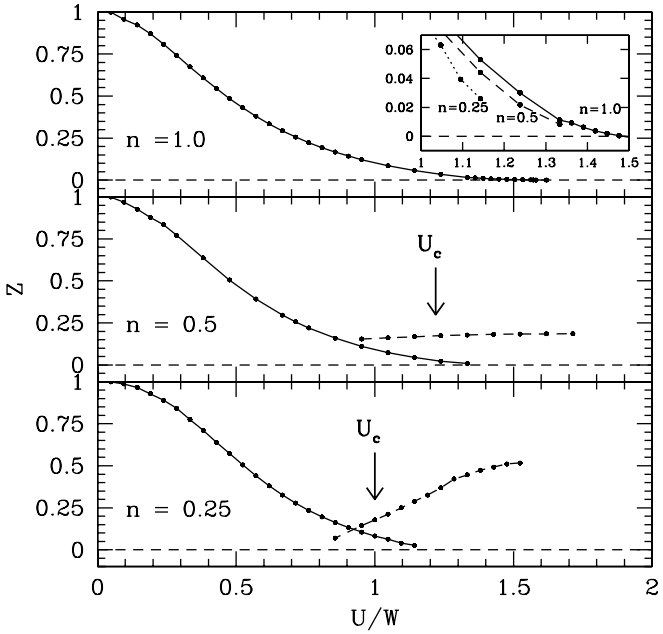

FIG. 1. The quasiparticle weight Z as a function of U for $n = 1$, $n = 0.5$, and $n = 0.25$. The solid and dashed lines join the solutions in the Fermi liquid and pairing phase, respectively. In the half-filled case the latter phase has always $Z = 0$. The first-order pairing transition is marked by a vertical arrow (for $n = 1$ the transition is second order and coincides with the vanishing of the metallic solution U_{c2}). In the inset, the metallic solutions in the proximity of their disappearance point U_{c2} are shown. The $n = 0.25$ (dotted line) and the $n = 0.5$ (dashed line) solutions have always nonvanishing Z, while the $n = 1$ solution (solid line) vanishes at U_{c2}.

in general, U_c has no relationship with the point in which the Z's of the two solutions coincide, so that Z has a jump at the pairing transition.

The above results give strong evidence for the finiteness of Z away from half filling. Nevertheless, extrapolating the QMC results of Ref. [6] down to $T = 0$, one would obtain, for U close to U_c, values of Z significantly larger than the exact diagonalization results reported here. The discrepancy is easily attributed to the relatively large temperatures used to extrapolate the $T = 0$ value. Further QMC calculations performed at lower temperatures indeed show a significantly smaller value of Z, which is in closer agreement with our values [11].

The finiteness of Z is a naively surprising result, since Z is usually interpreted as a sort of order parameter for the Mott metal-insulator transition at half filling. The half-filled case is, however, peculiar. In the general $n \neq 1$ case, the mapping onto the half-filled repulsive Hubbard model at finite magnetization, $m \neq 0$, indicates that in the Fermi liquid Z should stay finite because the low-energy (Kondo-like) resonance characterizing the metallic state cannot have a vanishing width due to the presence of a finite magnetic field h [12]. Also the Mott-insulating phase is different in the presence of a magnetic field. When $h = 0$ one has a pure Mott insulator with $Z = 0$, whereas, when h is large enough to align *all* the spins, one has a

completely filled uncorrelated band for, e.g., the up spins and one recovers the free-electron value $Z = 1$ [13]. It is then natural that, at intermediate values of the magnetic field, when $m \neq 1$ (i.e., at intermediate fillings in the attractive Hubbard model), Z assumes finite values. A further insight can be given by the atomic limit ($t = 0$), that well describes the strong-coupling limit $U \gg t$. At half filling, $\Sigma(\omega)$ diverges as $1/\omega$ for $\omega \to 0$, leading to $Z = 0$. On the other hand, away from half filling, the self-energy does not diverge at $\omega = 0$ and Z is always finite.

We now turn to the pairing transition in the grand canonical ensemble, where n is not fixed. We can divide the phase diagram in the U-n plane in four regions, as shown in Fig. 2: (a) $U < U_{c0} = 0.56W$, in which only the Fermi liquid solution exists for any density; (b) $U_{c0} < U < U_{c1}$, where the metallic solution exists only for densities from half filling to some intermediate value, and the insulating one exists only for small densities, and a coexistence region appears; (c) $U_{c1} < U < U_{c2}$, where the two solutions coexist at half filling and in an adjacent region, and the metallic solution disappears at some density; (d) $U > U_{c2}$, where only the insulating solution is present. In order to reveal a possible phase separation close to the pairing transition, we computed the density as a function of the chemical potential for various values of U. Phase separation occurs as soon as, for some range of densities, the density is not an increasing function of the chemical potential. If this is the case, a Maxwell construction determines the phase separation region, i.e., the densities of the phases in which the system separates. The results are shown in the schematic phase diagram of Fig. 2. In both the regions (a) and (d), as well as in the extreme point $U = U_{c0}$, the single phase is always stable with respect to phase separation. On the other hand, in the intermediate slices (b) and (c) of the diagram, the first-order phase transition is always accompanied by phase separation between two phases at intermediate densities. The system therefore displays the spatial coexistence of metallic and insulating domains at different densities in a finite region of densities around the pairing transition.

The existence of a pairing transition, its first-order character, and the finite value of Z could be expected on the basis of the known results for the repulsive model [13]. Nonetheless, the nature of the pairing phase and the mechanism leading to the disappearance of the Fermi liquid are less understood. The last part of this work is therefore devoted to the analysis of the evolution of the DOS as a function of U for fixed density, concentrating on the formation of the lower and upper Hubbard bands and on the disappearance of the quasiparticle Kondo resonance going from the metallic to the insulating solution.

For $U = 0$, the DOS is obviously the semicircular one, characteristic of a Bethe lattice, and the chemical potential moves inside this band to give the desired density. In the opposite atomic limit, we expect an insulating DOS with the broad upper and lower Hubbard bands. Since we work out of half filling, the two bands will have different weight. The effect of the attraction between the electrons is shown in Fig. 3 for the case $n = 0.75$. Starting from small values of U, the first visible effect of the interaction is a broadening of the whole spectrum, with the high-energy tails (top and bottom of the bands) moving away from the chemical potential. On the other hand, the total weight close to the Fermi level does not change much increasing U. Further increasing U, the effect is enhanced and the high-energy weight starts to separate from the low-energy feature. As a result, the featureless noninteracting DOS evolves into a well-structured function, that resembles the well-known result for $n = 1$, with three distinct features: a structure around the Fermi level, and two high-energy features,

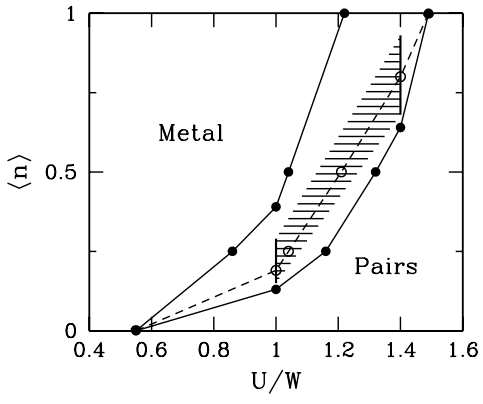

FIG. 2. Phase diagram in the U-n plane. The full dots are the calculated values of U_{c1} and U_{c2}, while the open dots are the pairing transition points. The thick vertical lines mark calculated phase separation intervals for $U/W = 1$ and 1.4, while the shaded area is a guide to the eyes.

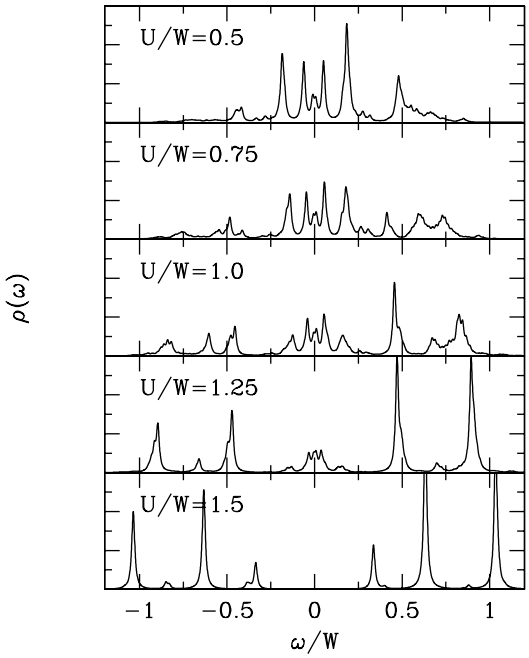

FIG. 3. Spectral density $\rho(\omega)$ for $n = 0.75$ and various values of U/W in the metallic phase (first four panels) and in the pairing phase (bottom panel).

analogous to the Hubbard bands. Since we have $n < 1$, the upper band has larger weight than the lower. Regions with significant depletion of spectral weight clearly separate the different features. Following the metallic solution beyond the transition point U_c, a finite spectral weight at the Fermi level is found for all coupling values up to U_{c2}, where the metal abruptly disappears. The breakdown of the Fermi liquid is not associated with a vanishing width of the Fermi level resonance, consistently with the results for the quasiparticle weight Z. The finite Z in the metallic solution is therefore associated with this quasiparticle feature at the Fermi level. As reported above, at $U = U_c < U_{c2}$, the metallic solution becomes energetically unfavored with respect to the pairing state. In that state the spectral function displays only the broad Hubbard bands, and is always gapped (although Z is finite). A similar behavior is present also for lower densities such as $n = 0.5$ and $n = 0.25$ (not shown), where all the transitions (disappearance of Fermi liquid and first-order pairing transition) move to lower U, and the interval in which three features coexist is narrower, but clearly present. In all cases, even if a loss of total spectral weight close to the Fermi level occurs, this weight never vanishes in the metallic phase and the transition to the pairing state is first order.

In conclusion, we have presented a complete characterization of the pairing transition in the normal phase of the attractive Hubbard model. For all densities $n \neq 1$, the pairing transition is intrinsically a first-order one, accompanied by a region of phase separation between a metallic and an insulating phase at different densities. The quasiparticle weight Z is always finite, and takes its minimum value at the transition point, where it jumps from a lower metallic value to a higher value in the pairing phase. Even following the metallic solution in the metastability region $U_c < U \leq U_{c2}$, Z never vanishes.

An analysis of the spectral function $\rho(\omega)$ shows that the finite Z in the metallic phase is associated with a quasiparticle peak at the Fermi level. The evolution of $\rho(\omega)$ is quite similar to the half-filled repulsive Hubbard model. A structure at the Fermi level is found all the way to the pairing transition, and two broad Hubbard bands develop and coexist with the Fermi-level feature. The neglect of superconducting symmetry breaking and the local nature of the pairing suggest that some care must be taken in carrying over our results to characterize the normal phase above T_c, particularly in systems (like cuprates) where the pairing has a nontrivial momentum structure. However, the above DMFT analysis provides interesting indications in two main regards. First of all, it shows that, for $U \simeq W$, preformed Cooper pairs and substantial pseudogap features can be obtained on a local basis (i.e., involving all momenta) even without invoking strong critical (i.e., at small q's) pair fluctuations in the proximity of a superconducting phase transition. This can even give rise to a phase of incoherent pairs, which, however, does not seem to be generically observed in the cuprates. At most one could argue that strongly bound incoherent pairs are formed near the $(\pm\pi, 0)$ and $(0, \pm\pi)$ points of the Brillouin zone, supporting a two-gap model for cuprates [14]. A second relevant outcome of DMFT analysis is the presence of coherent quasiparticles with a strong mass enhancement at intermediate coupling directly arising from the pairing interaction and coexisting with the high-energy pseudogap features. While the Hubbard-like high-energy features will survive the turning on of coherent pairing and will be present in the normal phase above T_c, the persistence of the relatively heavy quasiparticles above T_c is a more subtle issue. The renormalized quasiparticles are expected to survive to superconductivity only when T_c is less than their effective bandwidth, which is of the order ZW. This could leave a very narrow window around $U \simeq W$ where large pairing-induced mass enhancement is visible. Accordingly, by crossing $U \simeq W$, the superconducting transition will quickly evolve from a BCS-like instability of a Fermi liquid (with possibly critical pair fluctuation induced pseudogap on an energy scale less than ZW) to BE-like condensation of preformed pairs.

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