Dynamical Mean-Field Theory for Pairing and Spin Gap in the Attractive Hubbard Model

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We solve the attractive Hubbard model for arbitrary interaction strengths within dynamical mean-field theory. We compute the transition temperature for superconductivity and analyze electron pairing in the normal phase. The normal state is a Fermi liquid at weak coupling and a non-Fermi-liquid state with a spin gap at strong coupling. Away from half filling, the quasiparticle weight vanishes discontinuously at the transition between the two normal states.

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Fermi systems with a weak attractive interaction are Fermi liquids which undergo a phase transition into a superconducting state via the condensation of weakly bound Cooper pairs at a low critical temperature T_c. For a long time this weak coupling route to superconductivity, which is well described by the BCS mean-field theory [1], was distinguished almost dogmatically from Bose-Einstein condensation of bosons, until Leggett [2] showed that BCS superconductivity transforms smoothly into Bose-Einstein condensation of tightly bound pairs when the two-particle attraction between the fermions is increased gradually from weak to strong coupling. The size of the Cooper pairs shrinks continuously until spatially well separated bosons form, which undergo Bose condensation at a sufficiently low temperature. Nozières and Schmitt-Rink [3] have extended Leggett's analysis to lattice electrons and finite temperatures. Based on physical insight gained from a discussion of the weak and strong coupling limits and an approximate (T-matrix) treatment of the intermediate regime they concluded that the evolution from weak coupling to strong coupling superconductivity is indeed smooth.

The interest in the intermediate regime between the BCS and Bose-Einstein limits increased considerably after the discovery of high-temperature superconductors, which are characterized by Cooper pairs whose size is only slightly bigger than the average electron distance [4]. Much recent work has therefore been dedicated to the theory of Fermi systems with attractive interactions of arbitrary strength [5]. It was shown that sufficiently strong attraction or reduced dimensionality can lead to energy gaps even in the *normal* phase, which have been related to pseudogap phenomena in the cuprate superconductors [6].

In this work we analyze the formation of pairs in a Fermi system with arbitrary attractive interactions by solving the attractive Hubbard model within dynamical mean-field theory (DMFT) [7]. We show that the normal state is a Fermi liquid at weak coupling and a non-Fermi liquid state characterized by bound pairs and a spin gap at strong coupling, in qualitative agreement with Quantum Monte Carlo (QMC) studies of the two- and three-dimensional attractive Hubbard model [8–10]. At very low temperatures the transition between the Fermi liquid and the normal paired state is discontinuous.

In standard notation the Hubbard model for lattice fermions with a nearest neighbor hopping amplitude $-t$ and a local interaction U is given by

$$H = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \sum_{\sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{j}} n_{\mathbf{j}\uparrow} n_{\mathbf{j}\downarrow} . \qquad (1)$$

The attractive ($U < 0$) Hubbard model is a superconductor below a certain critical temperature $T_c(U,n) > 0$ for all U at any average density n, if the lattice dimensionality is above two [11]. At half filling ($n = 1$) the usual U(1) gauge symmetry becomes a subgroup of a larger SO(3) symmetry, and the superconducting order parameter mixes with charge density order. In two dimensions one expects a Kosterlitz-Thouless phase at low temperatures for all $U < 0$ and $n \neq 1$ [11].

In the weak coupling limit $U \to 0$ and dimensions $d > 2$ the attractive Hubbard model can be treated by BCS mean-field theory [3,11]. In the strong coupling limit $U \to -\infty$ the low energy sector of the model (excitation energies $\ll |U|$) can be mapped onto an effective model of hard-core lattice bosons with a hopping amplitude of order t^2/U and a repulsive nearest neighbor interaction of the same order [3,11]. These bosons undergo Bose condensation in $d > 2$ dimensions and a Kosterlitz-Thouless transition in two dimensions (for $n \neq 1$) at a critical temperature of order $t^2/|U|$.

For nearest neighbor hopping on a bipartite lattice the particle-hole transformation of spin-$\uparrow$ fermions

$$c_{\mathbf{j}\uparrow} \mapsto \eta_{\mathbf{j}} c^{\dagger}_{\mathbf{j}\uparrow}, \qquad c^{\dagger}_{\mathbf{j}\uparrow} \mapsto \eta_{\mathbf{j}} c_{\mathbf{j}\uparrow} , \qquad (2)$$

where $\eta_{\mathbf{j}} = 1$ (-1) for $\mathbf{j}$ on the A sublattice (B sublattice), maps the attractive Hubbard model at density n onto a repulsive Hubbard model at half filling with a finite average magnetization $m = 1 - n$ [11]. We will use this relation to compare with results known for the repulsive Hubbard model.

We have solved the attractive Hubbard model within DMFT [7]. In contrast to other (simpler) mean-field

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approaches, DMFT provides an exact solution of the model in the limit of infinite lattice dimensionality [12], since it captures local fluctuations exactly.

To convince ourselves that DMFT is a suitable approach for the weak to strong coupling crossover problem, let us first consider the limits. At weak coupling DMFT captures the complete BCS physics, since it contains the Feynman diagrams contributing to the BCS mean-field theory. At strong coupling, where the attractive Hubbard model maps to the hard-core Bose gas, DMFT reduces to the standard mean-field theory of the hard-core Bose gas [13]. Hence, Bose-Einstein condensation of preformed pairs is obtained at a critical temperature of order $t^2/|U|$ at large $|U|$.

Within DMFT the fluctuating environment of any lattice site is replaced by a local but dynamical effective field $\mathcal{G}_0$ [7]. The mean-field equations involve the calculation of the propagator $G(\tau) = -\langle \mathcal{T} c_\sigma(\tau) c_\sigma^\dagger(0)\rangle$ of an effective single-site Hubbard model coupled to the dynamical field $\mathcal{G}_0$, and a self-consistency condition relating G to the local propagator of the full lattice system. The lattice structure enters only via the bare density of states (DOS), as long as the translation invariance of the lattice is not broken. We have used the particularly simple self-consistency equations [7]

$$\mathcal{G}_0^{-1}(i\omega) = i\omega + \mu - (\epsilon_0/2)^2 G(i\omega), \qquad (3)$$

valid for a half-ellipse shaped density of states $D_0(\epsilon) = \frac{2}{\pi\epsilon_0^2}\sqrt{\epsilon_0^2 - \epsilon^2}$. Any other bounded DOS would yield qualitatively similar results. In the following we will set $\epsilon_0/2 = 1$. Susceptibilities such as the pairing and the spin susceptibility can also be computed from expectation values of operator products within the effective single-site problem. The DMFT equations can also be extended to superconducting or other symmetry broken phases [7]. In this work we focus, however, on normal state properties.

The effective single-site problem cannot be solved analytically. We have solved it numerically by discretizing the imaginary time interval and computing expectation values via the standard Hirsch-Fye algorithm [14].

We now present and discuss results from our DMFT calculation at quarter filling ($n = 1/2$). We do not expect that the results depend qualitatively on the density in the attractive Hubbard model, as long as n is finite. Only the particle-hole symmetric case $n = 1$ is special due to its larger symmetry group. Quarter filling is well below half filling but still high enough to see collective many-body effects, which are not obtained in the low-density limit.

The critical temperature T_c for the onset of superconductivity shown in Fig. 1 has been obtained from the pairing susceptibility in the normal phase, which diverges as the temperature approaches T_c from above. The critical temperature at half filling, where the superconducting state is degenerate with a charge-density wave state, has been computed within DMFT already earlier [15]. Note that correlations suppress T_c with respect to the BCS result even in the weak coupling limit, as expected [16]. At strong coupling $T_c(U)$ approaches the $1/U$ behavior described by the hard-core Bose gas limit. At intermediate coupling strengths, $T_c(U)$ varies smoothly, as predicted already by Nozières and Schmitt-Rink [3]. A comparison with a recent result for T_c obtained by combining the DMFT with a self-consistent T-matrix approximation (TMA) [17] shows that the latter approximation reproduces the correct qualitative behavior of $T_c(U)$, but fails quantitatively.

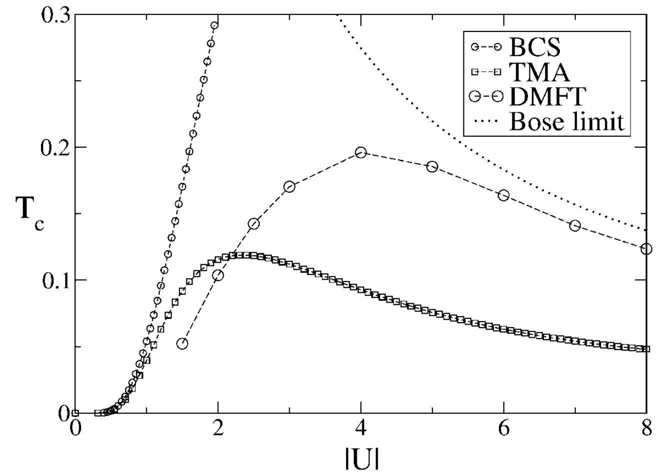

FIG. 1. Critical temperature T_c as a function of the coupling strength $|U|$ at quarter filling within DMFT, compared to T_c obtained from BCS theory and from the T-matrix approximation (TMA), respectively.

In the following, we discuss the weak to strong coupling crossover in the *normal* phase. We ignore the superconducting instability and study normal state solutions of the DMFT equations also below T_c. Of course these solutions do not minimize the free energy, but they could be stabilized by the field energy of a sufficiently strong external magnetic field.

At weak coupling the normal state of the system is a Fermi liquid with fermionic quasiparticle excitations. Besides numerical evidence this follows [18] from the analyticity of weak coupling perturbation theory for the effective single-site problem. By contrast, at sufficiently strong coupling $|U| \gg \epsilon_0$ and zero temperature all particles are bound in pairs, because a small kinetic energy cannot overcome a finite binding energy. Only short-ranged virtual breaking of local pairs occurs. At low finite temperatures $T \ll |U|$ only an exponentially small fraction of pairs dissociates.

A good measure for local pair formation is the density of doubly occupied sites $n_d = \langle n_{\mathbf{j}\uparrow} n_{\mathbf{j}\downarrow}\rangle$. For an uncorrelated state the density of doubly occupied sites is simply the product of the average density of up and down spin particles, i.e., $n_d^0 = n_\uparrow n_\downarrow = (n/2)^2$. An attractive interaction enhances n_d. In the limit of infinite attraction all particles are bound as local pairs such that $n_d \to n/2$. In Fig. 2 we show results for $n_d(T)$ for various U. Decreasing T from the high-temperature limit $n_d(T)$ first increases as

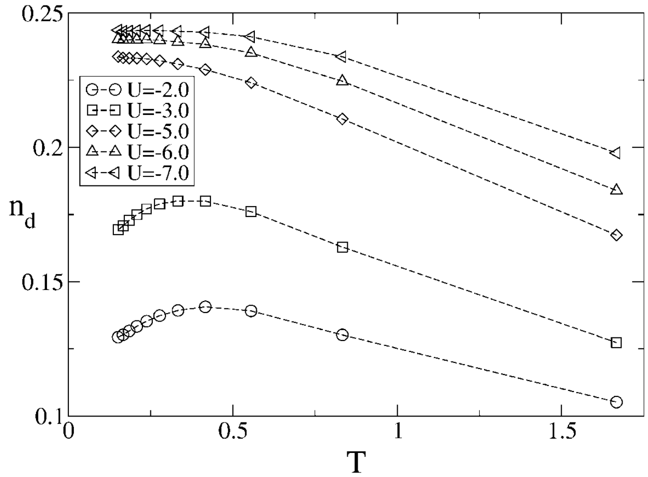

FIG. 2. Density of local pairs n_d as a function of temperature for various coupling strengths U at quarter filling.

a consequence of the attractive interaction. For small or moderate U, however, $n_d(T)$ slightly decreases again at low temperatures. This effect, which has also been obtained in the combined DMFT + TMA calculation [17], can be attributed to the kinetic energy, which tends to dissociate pairs if the attraction is not too strong. Note that in the pairing regime for stronger U the upturn in $n_d(T)$ at low temperatures is missing. The kinetic energy is not able to unbind pairs any more. A completely analogous (particle-hole transformed) behavior has been found in the DMFT solution of the repulsive Hubbard model at half filling [7].

The absence of fermionic quasiparticles in the pairing state at strong coupling also leads to a pronounced *spin gap*. In Fig. 3 we show our DMFT results for the temperature dependence of the spin susceptibility χ_s, for various coupling strengths. For a weak attraction the spin susceptibility increases monotonously for lower temperatures and then saturates at a finite value for $T \rightarrow 0$, as expected for a Fermi liquid. For strong coupling, however, χ_s decreases rapidly at low temperatures, as expected for a system where spin excitations are gapped. This gap, which has also been seen in QMC simulations of the two-dimensional [8,9] and three-dimensional [10] Hubbard model, is clearly due to the binding energy of pairs in the non-Fermi liquid state forming at strong coupling. For an intermediate attraction strength, pseudogap behavior seems to set in at intermediate temperatures, but for small T the susceptibility increases again and tends to a nonzero value (see $U = -4$). We expect that this behavior reflects the presence of a narrow quasiparticle band in the system, equivalent to the one known for the repulsive model near the Mott transition [7]. The self-consistent TMA fails to yield spin gap behavior in high dimensions [17], and yields only a rather weak suppression of χ_s in two dimensions [19].

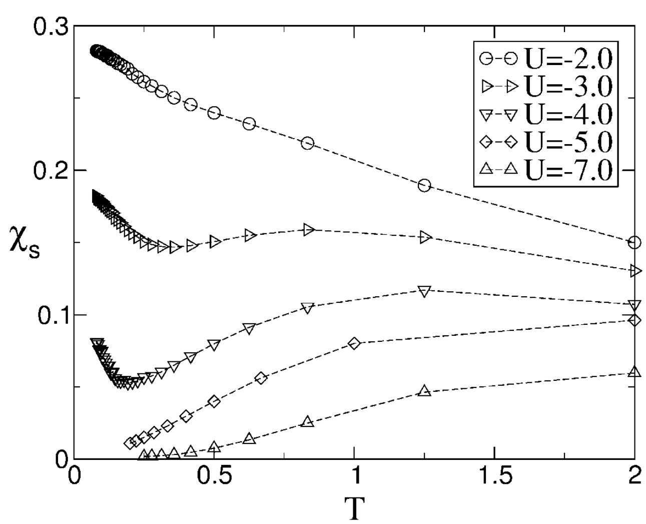

FIG. 3. Spin susceptibility χ_s as a function of temperature for various coupling strengths U at quarter filling.

Since the Fermi liquid state at weak coupling is qualitatively different from the bound pair state at strong coupling, there must be a sharply defined *pairing transition* at some critical attraction U_c at least in the ground state. At quarter filling we can estimate from our data $U_c \approx -2.5\epsilon_0$.

To see how the Fermi liquid breaks down upon increasing the attraction strength, we have computed the renormalization factor $Z(T) = [1 - \Sigma(i\omega_0)/i\omega_0]^{-1}$, where Σ is the self-energy and $\omega_0 = \pi T$ the smallest (positive) Matsubara frequency at temperature T. In Fig. 4 we plot $Z(T)$ as a function of T for various U at quarter filling (left) and at half filling (right). At quarter filling $Z(T)$ extrapolates to a finite positive value Z in the limit $T \rightarrow 0$, for any U. In the Fermi liquid phase Z has physical meaning, being the spectral weight for quasiparticles, the Fermi edge discontinuity in the momentum distribution function and, within DMFT, also the inverse mass renormalization. This meaning is of course lost in the bound pair state. Note that the finiteness of Z for all U does not imply that the system is a Fermi liquid for arbitrary interactions. A simple calculation shows that Z is finite even in the atomic limit $t = 0$, where the

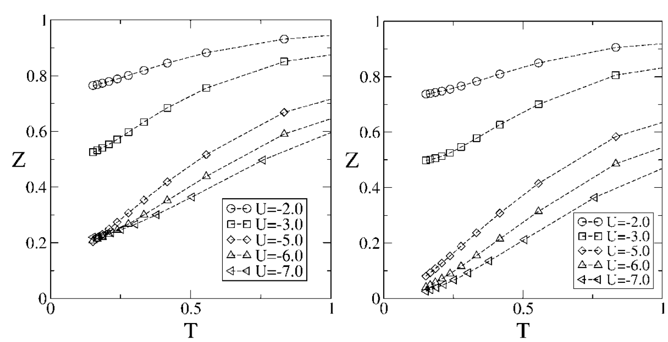

FIG. 4. $Z(T)$ as a function of temperature for various U at quarter filling (left) and half filling (right).

system is obviously not a Fermi liquid. An exception is the half-filled case, where $Z \to 0$ for $U \to U_c$, and $Z = 0$ for all $|U| \geq |U_c|$ (see Fig. 4) and in the atomic limit. For half filling the continuous vanishing of Z has been analyzed in much detail for the Mott transition in the repulsive Hubbard model [7], which is equivalent to the pairing transition in the attractive model by virtue of the particle-hole transformation (2). We thus conclude that the Fermi liquid phase disappears with a finite Z at electron densities $n \neq 1$, i.e., the quasiparticle weight disappears *discontinuously* at the pairing transition.

It is instructive to consider the low density limit $n \to 0$ for comparison. In that limit the bound pair state is stable once the attraction exceeds the threshold for two-particle binding U_c^0. For $|U| < |U_c^0|$ no bound states exist, and the particles move essentially freely, due to the low density, and Z is almost one even close to the transition.

Using the Hirsch-Fye algorithm it is hard to determine unambiguously whether there is a sharp phase transition at some critical $U_c(T)$ also at sufficiently low finite temperature or only a smooth (though steep) crossover, since the computation time increases rapidly at low temperatures. However, one can find an answer to this question by exploiting the equivalence of the attractive Hubbard model at generic densities and the half-filled repulsive Hubbard model with a finite magnetization. The latter model has been analyzed earlier within DMFT by Laloux *et al.* [20], who solved the DMFT equations with an exact diagonalization algorithm which is more efficient than the Hirsch-Fye algorithm at low temperatures. The results of their work imply that at very low temperatures a first order transition occurs in the attractive Hubbard model between a thermally excited Fermi liquid state and a thermally excited bound pair state.

In summary, we have shown that DMFT yields a transition from a Fermi liquid state at weak coupling to a non-Fermi liquid state with a spin gap at strong coupling in the attractive Hubbard model. Spin-gap behavior for *strong* attraction is obviously governed by *short-range* pair correlations which are captured by DMFT. Long-range superconducting fluctuations characteristic for low-dimensional systems are crucial for normal state gaps only at weaker coupling.

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