Energetic balance of the superconducting transition across the BCS-Bose Einstein crossover in the attractive Hubbard model

A. Toschi\textsuperscript{1,2}, M. Capone\textsuperscript{1,3}, and C. Castellani\textsuperscript{1}
\textsuperscript{1} Dipartimento di Fisica, Università di Roma “La Sapienza”, and INFN-SMC, Piazzale Aldo Moro 2, I-00185 Roma, Italy
\textsuperscript{2} Max Planck Institut für Festkörperforschung, Heisenbergstr. 1, 70569, Stuttgart, Germany
\textsuperscript{3} Istituto dei Sistemi Complessi del CNR, Via dei Taurini 19, I-00185, Roma, Italy

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We investigate by means of Dynamical Mean-Field Theory the crossover from BCS superconductivity to Bose-Einstein (BE) condensation of preformed pairs which occurs in the attractive Hubbard model by increasing the attraction strength. We follow the evolution of the two energy scales underlying the superconducting phenomenon, the gap $\Delta_0$ and the superfluid stiffness $D_S$, which controls the phase coherence. The BCS-BE crossover is clearly mirrored in a change in the hierarchy of these two scales, the smallest of the two controlling the critical temperature. In the whole intermediate-to-strong coupling region $T_c$ scales with $D_S$, while $T_C$ is proportional to $\Delta_0$ only in the BCS regime. This evolution as a function of the interaction qualitatively resembles what happens in the cuprates when the doping is decreased towards the Mott insulator.

This continuous change reflects also in the energetic balance at the superconducting transition. While, as it is well known, superconductivity is stabilized by a potential energy gain in the BCS regime, the strong-coupling superconductivity is made stable by a reduction of kinetic energy. Interestingly the intermediate-coupling region, where the maximum $T_c$ is achieved, behaves similarly to the strong-coupling regime, and its gain in kinetic energy is the largest as a function of the coupling. Since the integral of the optical conductivity is proportional to the kinetic energy, the above finding implies that the attractive Hubbard model can account qualitatively for the anomalous behavior of optical spectra around $T_c$, where an increase of spectral weight is observed in under and optimally doped cuprates, while the overdoped samples have a more standard behavior. This qualitative agreement is lost in the normal phase, specifically at strong-coupling, calling for the inclusion of strong correlation effects in the theoretical description.

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I. INTRODUCTION

High-temperature superconductors (HTSC) have attracted an unprecedented interest in the solid-state community, yet the number of open issues largely exceeds the number of generally accepted points. Among the latter, we can count the crucial role of strong electron-electron repulsion. This immediately raises the question of the competition and coexistence between this repulsion and the attraction between quasiparticles responsible of the superconducting phenomenon.

In this work, we make a step back, and we consider a simpler and more “phenomenological” question, that is the possibility to explain some features of the HTSC physics simply in term of a crossover between a conventional (BCS) superconductivity (characterizing the overdoped compounds) and a sort of strong-coupling Bose-Einstein (BE) superconductivity (in the underdoped region).\textsuperscript{1,2} A number of properties of the cuprates can in fact be qualitatively described in this framework. Notable examples are the intermediate values (\(~10 \div 20\) A) of the superconducting coherence length $\xi_0$ in optimally doped compounds,\textsuperscript{3,4} and the pseudogap phenomenology in the underdoped compounds,\textsuperscript{5,6} which can be ascribed to a “preformed pairs” phase, in which the superconducting order parameter has a finite amplitude, but it lacks phase coherence. The strongest connection with the physics of a BCS-BE crossover is perhaps the evolution with doping of the relevant energy scales controlling the stability of the superconducting condensate, namely the gap $\Delta_0$, which is proportional to the binding energy of the Cooper pairs, and the superfluid stiffness $D_S$, which represents the energy cost for phase fluctuations. In the underdoped compound there is a clear experimental evidence\textsuperscript{7,8} that $D_S < \Delta_0$ and $T_c$ is proportional to the “weak link of the chain” $D_S$ according to the so-called Uemura plot\textsuperscript{9,10}, whereas for higher doping a more conventional direct proportionality of $T_c$ on $\Delta_0$ is recovered.

However some obstacles arise trying to push further this line of thought. For instance, the unconventional $d$–wave symmetry of the order parameter, with the related presence of quasiparticle excitations down to zero energy, is known to strongly affect the low-temperature thermodynamic properties. In particular the nodal quasiparticles can dominate the low-temperature charge\textsuperscript{11,12} and thermal transport even in the strong-coupling regime, invalidating a purely bosonic description.

It is also intuitively hard to reconcile the BCS-BE crossover scenario with the relevance of strong correlation effects, which are naturally larger and larger when the doping is reduced and the Mott insulator is approached. Then, in the BCS-BE scenario, the attraction should be stronger in the same region where the repulsion is maxi-
of the critical temperature for the superconducting phase, investigated with DMFT in the past, but the attention was expected to lead to reliable results and allow for a demonstrative approach which neglects the spatial correlations. In this work we use for this purpose the Dynamical Mean-Field Theory (DMFT) exclusively to avoid superconducting solutions, a phase which is mainly on spectral properties. More precisely, the Hamiltonian of the attractive Hubbard model reads

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

where \( \langle ij \rangle \) indicates that the first sum is restricted to nearest neighbors sites only, \( c_{i\sigma}^{\dagger} (c_{i\sigma}) \) creates (destroys) an electron with spin \( \sigma \) on the site \( i \) and \( n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma} \) is the number operator; \( t \) is the hopping amplitude and \( U \) is the Hubbard on-site interaction. As it can easily seen, this model reproduces in the extreme weak- and strong-coupling limit the BCS and BE regime respectively, and allows to move in the whole crossover region, simply by adjusting a single parameter, the ratio \( U/t \).

From the theoretical point of view, a stringent test of the relevance of the crossover in the attractive Hubbard model for the cuprates has been mainly limited by the lack of reliable non-perturbative approaches able to follow the evolution from weak to strong coupling without a bias in some direction. In this work we use for this purpose the Dynamical Mean-Field Theory (DMFT), a non-perturbative approach which neglects the spatial correlations beyond the mean field level, but fully retains the local quantum dynamics, and becomes exact in the infinite coordination limit. The local nature of the attraction and the non-perturbative nature of DMFT are expected to lead to reliable results and allow for a democratic treatment of the different regimes and of the whole BCS-BE crossover.

The attractive Hubbard model has been already investigated with DMFT in the past, but the attention was focused mainly on the normal phase or on the determination of the critical temperature for the superconducting transition, with the recent exception of Ref. 14, where the BCS-BE crossover at \( T = 0 \) is analyzed using iterated perturbation theory as an impurity solver, but the focus is mainly on spectral properties. More precisely, by explicitly avoiding superconducting solutions, a phase transition has been found both at finite and at zero temperatures15,16 between a metal and a “paired” phase, i.e., a collection of independent pairs without the superconducting phase coherence. This paired phase represent the “negative-U” counterpart of the paramagnetic Mott insulator found for the repulsive Hubbard model15,16.

With the present work we complete the DMFT analysis of this model reported in the Refs. 15,16,17 with a careful investigation of the properties of the superconducting phase, certainly stable at low temperatures. Although the onset of the superconductivity smooths the abrupt changes observed in the low-temperature metastable normal phase, and the evolution of the superconducting phase as the coupling is increased is a smooth crossover, the way in which the energetics changes in this process is extremely interesting. We fully characterize the crossover from BCS to BE superconductivity, and we establish that the intermediate regime, where the maximum \( T_{c} \) is obtained, shares the behavior of the strong-coupling, BE superconductivity. In particular, this means that the “optimal” superconductor is stabilized by a kinetic energy gain, as it is expected in the bosonic regime, as opposed to the standard potential energy stabilization characteristic of weak-coupling superconductivity.

The paper is organized as follows: Sec. II briefly describes the DMFT for an s-wave superconductor, Sec. III is devoted to the evolution of the superfluid stiffness and the gap as a function of the interaction, Sec. IV presents the energetic balance at the superconducting transition, and the relation with optical measurements. Sec. V is dedicated to concluding remarks.

II. METHOD

In this section we will briefly introduce DMFT and some aspects related to the study of superconducting solutions. DMFT maps a quantum lattice model onto an impurity model whose hybridization function (usually called Weiss field in analogy with classical mean-field theories) is determined by means of a self-consistent equation. The latter equation contains the information about the original lattice only through the non-interacting density of states. In our case is mapped onto an Anderson model with attractive coupling. In order to describe the superconducting phase, the bath presents superconducting terms leading to an anomalous Weiss field

\[ H_{AM} = \sum_{l, \sigma} \left[ c_{l\sigma} c_{l\sigma}^{\dagger} + V_{l} (c_{l\uparrow} d_{\sigma} + h.c.) + \Delta_{l} (c_{l\sigma} c_{l\sigma}^{\dagger} + h.c.) \right] + H_{loc} \]  

where \( H_{loc} = -U (n_{0\uparrow} - \frac{1}{2}) (n_{0\downarrow} - \frac{1}{2}) - \mu n_{0} \) is the on-site term, and the chemical potential \( \mu \) is adjusted to fix the particle density on the impurity site (in our calculations we always fix \( n = 0.75 \)) as a generic density out of half-filling, as done in Refs. 10,17.

From the impurity model we compute the normal and anomalous Green’s functions, \( G(\tau) = -(TC_{l}(\tau)c_{l}(0)) \) and \( F(\tau) = -(TC_{l}(\tau)c_{l}^{\dagger}(0)) \), which are used to build the matrix \( G(i\omega_{n}) \) in Nambu-Gor’kov formalism. Analogously one can define a matrix of Weiss fields whose
diagonal $G^0((i\omega_n)^{-1}$ and off-diagonal $F^0((i\omega_n)^{-1}$ elements are related to the parameters appearing in $\Sigma$ by

$$G_0^{-1}(i\omega_n) = i\omega_n + \mu + \sum_{l=1}^{n_s} V_l^2 \frac{i\omega_n + \epsilon_l}{\omega_n^2 + \epsilon_l^2 + \Delta_l^2}$$

$$F_0^{-1}(i\omega_n) = -\sum_{l=1}^{n_s} V_l^2 \frac{\Delta_l}{\omega_n^2 + \epsilon_l^2 + \Delta_l^2}. \quad (3)$$

The two above quantities also define the local self-energy matrix

$$\Sigma(i\omega_n) = G_0^{-1}(i\omega_n) - G^{-1}(i\omega_n). \quad (4)$$

The self-consistency relation relates the two above quantities to their normal-state counterparts as soon $\Delta_l = 0$ for each $l$.

The inclusion of local quantum fluctuations rules out the possibility to analytically solve Eqs. (2) - (5), and requires numerical (or approximate) solutions of the Anderson impurity model. Here we adopt Exact Diagonalization (ED) as the impurity solver. Thus, we discretize the Anderson model, by truncating the sums in Eqs. (2) and (5) to a small finite number of levels $N_s$. It has been shown that extremely small values of $N_s$ provide really good results for thermodynamic properties and reliable results for spectral functions. Here we use both the Lanczos algorithm (at zero temperature) and the finite temperature algorithm in its simplest version, which requires the full spectrum of the Hamiltonian matrix. To obtain the full spectrum of the Hamiltonian, we use the Lanczos algorithm (zero temperature) and the finite temperature algorithm in its simplest version, which requires the full spectrum of the Hamiltonian matrix. To obtain the full spectrum of the Hamiltonian, we use the Lanczos algorithm (zero temperature) and the finite temperature algorithm in its simplest version, which requires the full spectrum of the Hamiltonian matrix. To obtain the full spectrum of the Hamiltonian, we use the Lanczos algorithm (zero temperature) and the finite temperature algorithm in its simplest version, which requires the full spectrum of the Hamiltonian matrix. To obtain the full spectrum of the Hamiltonian, we use the Lanczos algorithm (zero temperature) and the finite temperature algorithm in its simplest version, which requires the full spectrum of the Hamiltonian matrix.
in the weak-coupling regime, but also for sizable interaction, as shown in Fig. 1 for $U = 2D$, where $D_S/D_N$ at $T = 0$ turns out to be less than 0.01. This means that it is possible to identify $D_S(T = 0)$ with $-\langle E_{\text{kin}} \rangle$ in a wide range of couplings. It is clear that this results depends on the neglect of small-momentum collective modes, which can deplete the condensate. It is worth noting that the presence of a frequency-dependent self-energy and of an incoherent part of the Green’s function does not lead to a reduction to a depletion of $D_S$, differently from what happens, for instance, for impurity scattering.

We now come to the evolution of the energy scales inherent to the superconducting phase as a function of the interaction. Our results are summarized by Fig. 2 where the superconducting gap $\Delta_0$, the superfluid stiffness $D_S$ and the critical temperature $T_c$ are plotted as a function of the ratio $U/D$. $\Delta_0$ is smallest in the weak-coupling regime, and the superfluid stiffness becomes the lowest scale in strong-coupling. It is natural that the system becomes superconductor only when the pairs are formed and they have phase coherence, namely when the temperature is lower than both the gap scale and the superfluid stiffness scale. Therefore the critical temperature is lower than both the gap scale and the superfluid stiffness scale in strong-coupling. It is natural that the system condensation of preformed bosons already at a moderate values of the interaction.

On the other hand, the attractive Hubbard model, at least in our DMFT framework, cannot reproduce the deviations from the Uemura plot recently observed in the cuprates. More specifically an evident “re-entrance” of the curve $T_c(D_S)$ has been observed in many overdoped compounds, and its shape appears to be strongly material dependent. In our calculation at small $U$, where $D_S \sim -\langle E_{\text{kin}} \rangle$, the superfluid stiffness is a monotonically decreasing function of the interaction, and does not show the experimentally observed re-entrance.

In order to push a little bit further the comparison with the most recent experimental data, it is useful to recast our DMFT results for the “Uemura plot” rescaling $T_c$ with the superconducting gap $\Phi_0$ in the single particle spectrum, as done by Tallon et al., in order to single out as much as possible the nonstandard behavior of $T_c$. The experimental $T_c/\Phi_0$ is found sub-linear in $D_S$ in the underdoped regime, while it is slightly super-

![FIG. 1](image1.png)

**FIG. 1:** (Color online) Temperature dependence of the superfluid stiffness $D_S$ and of the normal component $D_N$ at $U = 2D$ (just before the maximum $T_c$) compared with the diamagnetic term $-\langle E_{\text{kin}} \rangle$.

![FIG. 2](image2.png)

**FIG. 2:** (Color online) Superconducting energy scales (in unit of $D$) ($\Delta_0$ and $D_S$ have been normalized to be directly comparable with $T_c$ in the asymptotic regimes). The two energies cross at intermediate coupling at $U \sim D$, well before the maximum $T_c$ dome ($T_c$ is taken from Ref. [10]).
FIG. 3: (Color online) Uemura plot in the attractive Hubbard model. The direct proportionality between $D_S$ and $T_c$ in the strong-coupling limit is evident on the left side of the figure, corresponding to $U > 2.4D$.

linear at higher doping (with a not universal tail in most overdoped compounds). We notice that, beyond the BCS regime $\Phi_0$ can be different from the order parameter $\Delta_0$ that we have introduced before. Here $\Phi_0$ is evaluated directly as the gap in the density of states. The difference between the two quantities varies up to 30%.

Our results are summarized in Fig. 4 where one can note the presence of a wide region of a sub-linear behavior of $T_c/\Phi_0$ on the left-side of the figure, which corresponds to the intermediate-to-strong coupling regime in fair agreement with Ref. [28]. Also a partial of a super-linear behavior appears on the right-hand side of our plot. The observed behavior of $T_c/\Phi_0$ is therefore captured by our simple BCS-BE crossover, without invoking more involved explanations [28].

The evolution of energy scales we have discussed in this section is reflected in an increased role of phase fluctuations as the coupling grows. As we have mentioned in the introduction, those fluctuations may have in principle relevant effects on the superconducting phase, in which finite dimensionality effects beyond DMFT can be important, possibly destroying the superconducting ordering. In DMFT, indeed, phase fluctuations at large $q$ are properly taken into account, while the small $q$ collective modes are neglected. In Ref. [29] it is argued that superconductivity is destroyed by phase fluctuations for $U$ larger than a critical value due to the small charge compressibility $\kappa = \partial n/\partial \mu \propto 1/U$ derived within a phase-only effective theory based on the atomic limit. Since $\kappa$ measures the inertia of the system against the dynamic phase fluctuations, a small value would permit large zero-point fluctuations, eventually destroying phase coherence. On the other hand, an alternative derivation of a phase-only action within one-loop expansion gives instead $\kappa \sim 2U/D^2$, therefore increasing with $U$.

Even if DMFT neglects finite-dimensionality effects and cannot therefore treat the physics of the Goldstone modes associated with the phase-fluctuations, we can use this approach to evaluate the coefficients appearing in the phase-only effective theories. The lack of bias towards weak or strong coupling of DMFT should allow us to discriminate between the two derivations. The results shown in Fig. 5 clearly display that $\kappa$ grows linearly with $U$ at strong coupling in agreement with Ref. [29]; the cost of dynamic phase fluctuation at $q \approx 0$ tends to increase in the large $U$ limit, leaving the superconducting phase stable, in contradiction with Ref. [29]. A more complete description of the phase-fluctuations would require the calculation of all the phase-only theory coefficient, including the anharmonic ones. This issue is beyond the

FIG. 4: (Color online) Rescaled “Uemura-plot” (following Ref. [28]) for the attractive Hubbard model. We have plotted the $T_c$ divided by the gap $\Phi_0$ as a function of the superfluid density. It is evident the sub-linear behavior of $T_c/\Phi_0$ in the intermediate-to-strong coupling regime, which mirror rather well the data of Ref. [28] for several underdoped or optimally doped cuprates.

FIG. 5: (Color online) Charge compressibility in the superconducting phase at $T << T_c$. The DMFT data are compared respectively with the strong-coupling behavior from the phase-only action of Ref. [25] and with the noninteracting value.
IV. ENERGETIC BALANCE OF THE SUPERconducting PHASE AND OPTICAL SUM RULE

The characterization of the superconducting phase can be made more concrete by studying the temperature behavior of the kinetic ($E_{\text{kin}}$) and the potential ($E_{\text{pot}}$) energies. From one side this analysis allows to evaluate separately all the energetic contributions which characterize the mechanism for the stabilization of the superconducting long range order across the BCS-BE crossover. On the other hand, since in a lattice system the frequency integral of the optical conductivity $\sigma(\omega)$ can be related to the kinetic energy of the carriers, our calculations allow for a direct comparison with the optical measurements on the cuprates.

A. Kinetic and Potential Energy behavior

The calculation of both potential and kinetic energies is quite straightforward in DMFT, since it only involves local quantities. This is evident for the potential energy, because by definition it is proportional to the local density of double occupancies $n_d = (\sum_{i} n_{i\uparrow} n_{i\downarrow})$

$$E_{\text{pot}} = - Un_d. \quad (9)$$

As far as $E_{\text{kin}}$ is concerned, exploiting the simplified form of the self consistency equation for the Bethe lattice we can derive the following expression

$$E_{\text{kin}} = t^2 T \sum_{i\omega_n} [G(i\omega_n) G^*(i\omega_n) + G^*(i\omega_n) G(i\omega_n)]$$

$$- 2F(i\omega_n) F(i\omega_n)], \quad (10)$$

which shows that also the kinetic energy can be expressed only in terms of the local (normal and anomalous) Green function.

In Fig. 6 we report the kinetic energy and potential energies for $U = 0.8D, 2.4D$ and $3.6D$, chosen as representative of the BCS, the intermediate and the BE regimes, as a function of the temperature. The onset of the superconductivity is always marked by an abrupt change in the concavity of $E_{\text{kin}}(T)$ and $E_{\text{pot}}(T)$. The energetic balance of superconductivity displays instead clear differences between the various regimes. At $U = 0.8D$ the onset of superconductivity is accompanied by a slight loss in the kinetic energy ($\Delta E_{\text{kin}} = E_{\text{kin}}(0) - E_{\text{kin}}(T_c) = +0.003D$), and potential energy gain ($\Delta E_{\text{pot}} = E_{\text{pot}}(T = 0) - E_{\text{pot}}(T_c) = -0.008D$), as in standard BCS theory. On the other hand, both at $U = 2.4D$ and $U = 6.4D$ the superconducting phase is characterized by a lower value of $E_{\text{kin}}$ and a loss of potential energy is observed below $T_c$.

Such changes in the energetic balance at the superconducting transition clearly highlight the different mechanisms stabilizing superconductivity in the two regimes. In the BCS limit superconductivity coincides with pair formation, which determines a gain in potential energy and a consequent loss in kinetic energy. In the opposite BE regime, the electrons are paired at a high temperature of order $U$, but a true long-range superconducting order can take place only when phase coherence establishes between pairs. Therefore $T_c$ is associated to a gain in kinetic energy, while a small fraction of the potential energy gained with pair formation is lost at $T_c$.

More interestingly, our calculations indicate that already at intermediate $U$ the “strong-coupling” mechanism is taking place, and superconductivity is associated with a consistent kinetic-energy gain, such as the one observed in the optimally doped cuprates (see next sub-section). The kinetic energy gain turns out to be maximum at intermediate $U/D$, where the highest $T_c$ is achieved. The overall picture is drawn in Fig. 7 where we have reported the variation of the kinetic $\Delta E_{\text{kin}}$, the potential $\Delta E_{\text{pot}}$ and the total energy $\Delta E_{\text{tot}}$ between $T = T_c$ and $T = 0$ for a number of interaction values. From these data one can easily see that (i) the typical BCS feature of an increasing $E_{\text{kin}}$ below $T_c$ is rapidly lost (approximatively for $U \sim D \sim U_h$), in agreement with the discussion of the previous section; (ii) an intermediate region exists, in which the onset of the SC phase is associated with a gain of both potential and kinetic energy; (iii) the BE regime is effectively reached for $U$ larger than $1.8D$ (hence before reaching the maximal critical temperature), where superconductivity is stabilized.
by kinetic energy.

It is also worth noting in Fig. 7 that the variation of the total energy $\Delta E_{\text{tot}}$ has approximately the same dome-shape behavior of the $T_c$ dependence on $U$. It is tempting then, to consider this value as a measure of the condensation energy $E_c = E_{\text{ion}}(T = 0) - E_{\text{ion}}(T = 0)$ of the superconducting phase. This identification works well only if one can assume a small variation of $E_{\text{ion}}^S(T)$ between $T = T_c$ and $T = 0$, an assumption which holds both at small (due to the small value of $T_c$) and at intermediate-large $U$ (where both $E_{\text{kin}}$ and $E_{\text{pot}}$ are almost constant in temperature above $T_c$). However this is not the case for $U \sim 1 \div 2$ D, where a strong temperature dependence of $E_{\text{kin}}(T)$ (and of $E_{\text{pot}}(T)$) in the normal phase is found, because of the presence of a strongly renormalized quasiparticle excitation at the Fermi level. Within DMFT the situation is even more involved for $U_{c1} \sim 2.2D < U < 2.9D \sim U_{c2}$ where a coexistence between metallic and insulating solution is found and the temperature dependence of $E_{\text{kin}}$ and $E_{\text{pot}}$ in the normal phase below $T_c$ is subject to extremely abrupt changes. However this is a peculiar feature of the DMFT treatment of the Hubbard model which could not be so relevant when comparing our result with the experimental findings, also because these features of the Hubbard physics occur at temperatures much smaller than $T_c$.

### B. Comparison with the optical measurements

The integral over all the frequencies of the real part of the optical conductivity in a lattice model is related to the second order derivative of the free particle dispersion according to the following equation,

$$
\int_0^{+\infty} \sigma_{xx}(\omega) \, d\omega = \frac{\pi e^2}{2NV} \sum_{k,\sigma} \frac{\partial^2 \epsilon_k n_{k,\sigma}}{\partial k^2_x} (11)
$$

and the effect of the interactions is hidden in the values of the momentum distribution function $n_{k,\sigma}$. Here $\langle E_{\text{kin}} \rangle = \frac{1}{N} \sum_{k,\sigma} \epsilon_k n_{k,\sigma}$, $a$ the lattice spacing, $d$ the dimension of the system considered, and $V$ the unit-cell volume. The second equality, which holds for nearest-neighbor hopping only, implies that the kinetic energy data in Figs. 6 and 7 can be compared directly with the optical spectral weight of the conduction band in the cuprates.

The experimental results for the low-energy behavior of the spectral weight behavior in the HTS have been the object of a recent intense debate, and consensus has been reached about a few general points. In all the cuprates a sensible enhancement of low-energy spectral weight $W(T) = \int_0^{\Omega_C} \omega \sigma_{xx}(\omega, T)$ ($\Omega_C$ being a frequency cut-off of the order of 1 eV, which is the plasma frequency for those materials), is observed when lowering the temperature. In the superconducting phase, underdoped (UD) and the optimally (Opt) doped samples behave differently from the overdoped (OD) ones. More precisely, in the UD-Opt compounds below $T_c$ an upward bump is observed with respect to the normal phase behavior, in contrast with the decreasing of $W(\Omega_C, T)$ observed in OD samples.

The gain of kinetic energy per Cu atom $\Delta E_{\text{kin}} = E_{\text{kin}}(T_c) - E_{\text{kin}}(0)$ in UD-Opt BSCCO can be estimated using $d\sigma_{xx}(\omega, T)$ as $\Delta E_{\text{kin}} = -(0.5 \div 1) \text{ meV}$. Quite noticeably, this value of $\Delta E_{\text{kin}}$ is much higher than the condensation energy for the same materials, estimated as $E_c \sim 0.1 \text{ meV}$ on the basis of the specific heat measurements.

According to our DMFT results, the bump of $W(\Omega_C, T)$ observed below $T_c$, can be qualitatively understood in the framework of the BCS-BEC crossover. More specifically the hypothesis of an intermediate-to strong coupling description of the superconductivity in the UD-Opt region appears to fit well with the observed enhancement of the low-frequency spectral weight below $T_c$, whereas the disappearance of the upward bump in the OD cuprates is perfectly compatible with a weak-coupling superconductivity. It is interesting therefore to check to what extent is possible to push forward such an analogy with the properties of the real systems.

We can try to establish a comparison with the experimental data by choosing the value of the semi-bandwidth $D$ of the attractive Hubbard model in order to reproduce the maximum value $T^{\text{max}}_c$ of a $T^{\text{max}}_c$ of 90 $\sim 100$ K is obtained with $D \sim 1000 K \sim 100 \text{ meV}$. The theoretical values for $|\Delta E_{\text{kin}}|$ and $|\Delta E_{\text{tot}}|$ (that we take as an estimate of $E_c$) are respectively $4 \div 8$ meV and $2 \div 4$ meV,
larger by less than one order of magnitude than the experimental values in the underdoped HTSC. It is anyway remarkable that the DMFT of the attractive Hubbard model correctly predicts the qualitative trend of a condensation energy which is only a fraction of the kinetic energy gain.

As soon as the temperature exceeds $T_c$ and we enter the normal phase, our calculation ceases to properly describe the experimental results. The $T^2$ behavior of $E_{kin}$ is in fact found only in the BCS region, as shown by the $U = 0.8D$ data of Fig. 4 and it completely disappears in the intermediate-to-strong coupling regime: no relevant variation of $E_{kin}(T)$ is found at $U = 2.4, 6.4D$ in a wide temperature range above $T_c$. The inadequacy of the present approach to describe the experimental findings in the normal phase has different origins. A first reason is the freezing of spatial fluctuations characteristic of single-site DMFT. It is indeed reasonable to expect a role of short-range fluctuations at least at strong coupling. In this limit the attractive Hubbard model can be mapped in an effective “pseudospin” hamiltonian, and the kinetic energy is given basically by nearest-neighbor correlations between the pseudospin operators, i.e., the local pairs and the empty sites. The temperature dependence of these correlations is poorly described by DMFT at large $U/D$. The relevance of this effect can tested using cluster extensions of DMFT\cite{13, 14}, where the short-range spatial correlations are included.

There is however a more basic reason for the inadequacy of the attractive Hubbard model to capture the temperature behavior of the normal phase of the cuprates, which is the inability to properly describe the approach to the Mott insulator as the doping is reduced. The underdoped region is indeed almost universally believed to be dominated by the physics of a doped Mott insulator, with strongly renormalized quasiparticles. On the other hand, the strong-coupling region of our BCS-BE framework is certainly a “correlated” regime, with renormalized quasiparticles, but the interaction is simply the attractive one, which does not lead to the Mott insulating state. Indeed in a recent work\cite{30, 31} it has been explicitly shown that the physics of a doped Mott insulating system, with its associated band-narrowing, may represent the natural explanation for the strong temperature dependence of the spectral observed in the normal phase of the cuprates.

V. CONCLUSIONS

In this paper we have performed a detailed investigation of the physics of superconducting phase in the attractive Hubbard model both at zero and at finite temperature. The approach used here, namely the Dynamical Mean Field theory, is completely non-perturbative allowing for a treatment of the superconducting phase properties, which is not tied in principle either to the weak-coupling (BCS) or to the strong-coupling (BE) regime.

In particular we have investigated the behavior of the energy scales relevant for the superconductivity as a function of the pairing interaction $U$. We have found that the evolution of the superfluid density $D_S$ and the superconducting gap $\Delta_0$ displays a clear crossing in the intermediate coupling regime, which is reminiscent of what is found experimentally in the phase-diagram of HTSC for different doping levels. In the weak-coupling region the BCS picture works well and the superconductivity is controlled by the binding energy of the Cooper pairs $\Delta_0$: on the contrary when the pairing interaction is high the superconductivity becomes essentially a phenomenon of superfluidity of preformed local pairs. This is clearly witnessed by the direct proportionality found in this regime between $T_c$ and $D_S$, and showed in a sort of “Uemura-plot” for the attractive Hubbard model. We also consider explicitly the problem of superconductivity suppression due to phase fluctuations in the hydrodynamic regime, which is usually neglected in a DMFT framework. Our DMFT calculation of the compressibility indicates that, contrary to the claim of Ref.\cite{30}, the phase-fluctuation effects do not destroy superconductivity, even for extremely large values of $U$.

The analysis of the superconducting phase properties in the attractive Hubbard model has been then further enriched by considering the energetic stabilization of the superconductivity and the f sum-rule of the model. Our results clearly show a remarkable difference in the energetic balance responsible for the stabilization of superconducting order when moving along the BCS-BE crossover. While in the weak-coupling regime the onset of superconductivity is associated to a gain of potential energy and a slight loss in kinetic energy as it is expected in a BCS picture, already in the intermediate coupling at $U \approx D$ and specifically in proximity of the maximum of the $T_c$ dome, the situation is completely reversed. Here, and for higher values of $U$, the stabilization of the superconductivity is due to a marked reduction of $E_{kin}$, while a smaller (but sizable) loss of potential energy is observed. Therefore the onset of superconductivity is clearly distinct from Cooper pair formation already for moderate values of the pairing interaction.

The energetic balance at the superconducting transition finds a direct experimental counterpart in the optical measurements, since the integral of the optical conductivity is proportional to the kinetic energy itself. Our results can be rephrased in this terms, so that in weak-coupling a slight reduction of the optical sumrule is found in our calculation at the superconducting transition, while a relevant enhancement of the sumrule is observed for $T < T_c$ in the whole intermediate-to-strong coupling region. This scenario is actually realized in optical measurements in the HTSC cuprates as a function of doping, with overdoped samples behaving more or less as standard BCS superconductors, and underdoped one, characterized by a gain in kinetic energy\cite{32, 33, 34}.

A more quantitative comparison with the experiments
reveals that the variations of both kinetic energy and condensation energy between $T = 0$ and $T_c$ are reasonably well reproduced by our model, which also correctly predicts that a sizable fraction of the kinetic energy gain is canceled by the potential energy loss, leading to a condensation energy significantly smaller than the kinetic energy gain, as it indeed happens in the HTSC. It must be noticed that our calculation tends to overestimate both kinetic energy gain and condensation energy. However, the main limitation of the attractive Hubbard model in this context is the inability to capture the $T^2$ enhancement of the spectral weight in the normal phase above $T_c$. The main reason for this disagreement is likely the complete neglect of the strong repulsive interactions characterizing the underdoped cuprates close to the Mott state.

An important outcome of our analysis is that the optimal critical temperature is obtained for an interaction strength well inside the BE region. This finding is in good agreement with previous calculations of the pseudogap temperature $T^*$ extracted from the spin susceptibility and specific heat, where the $T^*$ is significantly larger than $T_c$ at optimal interaction, but it is in contrast with experiments in Bismuth and Yttrium based cuprates, where $T^*$ tends to vanish close to optimal doping. It is interesting to notice that this discrepancy seems to disappear if we fix the attraction strength $U$ and follow the BCS-BE crossover by varying the half-bandwidth $D$, and measuring energies in units of $U$. Such a rescaling is meant to roughly describe a situation in which the crossover from BCS to BE is due to a shrinking of the coherent band due to strong repulsive correlation effects which are stronger and stronger as the Mott insulator is approached, while the attraction, which we might think to arise from antiferromagnetic superexchange for the sake of definiteness, is basically unrenormalized in the same process.

As shown in Fig. 8, the maximum critical temperature now occurs for $U \simeq D$, at the boundary of the BCS region, where the pseudogap is small. However this different perspective, in which the optimal $T_c$ moves closer to the BCS region is in contradiction with the experimental evidence of a kinetic-energy driven superconductivity around optimal doping, which is qualitatively obtained in the BE regime.

As a summary of our results, we can draw some final considerations on the the connection of the BCS-BE crossover scenario and the physics of the HTSC: several qualitative feature of the HTSC properties (as the crossing of the hierarchy of $D_S$ and $\Delta_0$, the Uemura plot, ...) can be actually captured within a purely attractive description. However, as a general trend, it provides too high estimation of the values of many thermodynamic quantities as the kinetic energy variation below $T_c$ and the condensation energy. At the same time the purely attractive description fails in reproducing the magnitude of the temperature dependence of the optical spectral weight above $T_c$, calling for the inclusion of strong correlation effect and suggesting that a closer agreements with the physics of the cuprates may be obtained by applying the attractive Hubbard description, or more generally the BCS-BE crossover picture, only to the narrow quasiparticle excitations characteristic of a doped Mott insulator. Models in which explicit attractive and repulsive interaction are present are natural candidates to explore this scenario.

After completion of this work, we became aware of recent Cellular DMFT results by Kyung, Georges and Tremblay (cond-mat/0508645), where it is proposed that the inclusion of short range correlations beyond single-site DMFT makes the evolution on the normal state continuous, and the zero-temperature energetic balance of the superconducting transition is studied.

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