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SUPERCONDUCTORS: A PARTICULAR OVERVIEW

Phase separation as a possible scenario for high T_c superconductors: a particular overview

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Abstract

After a few considerations on the present understanding of the normal and superconducting phases in high temperature superconductors, we discuss phase separation as a possible scenario for developing pairing and an anomalous normal state. A specific model is discussed, which allows for phase separation arising from two distinct mechanisms associated to spin and charge degrees of freedom. The two physical mechanisms may drive density fluctuations along two distinct channels, so that the variation of relative weight of these two types of fluctuations may produce a gradual change with doping of the characteristics of the metal in the normal phase. On the other hand, superconductivity can take place over an extended range of doping as a consequence of the attractive forces produced by the tendency to phase separate driven by the combination of the two mechanisms.

I. INTRODUCTION

The specific order associated with a superfluid transition, i.e. the macroscopic occupation of a "single-particle state", has found its complete formulation only in two limiting cases: i) The Bose-Einstein condensation with onset at the degeneracy temperature of the preexisting bosons ($k_B T_c^{BE} \simeq \hbar^2 n^{2/d} / m^*$, $d > 2$); ii) The BCS theory leading to the coherent superposition of pairs of fermions in k space with large spatial overlap.

The condensation criterion associated to the Off-Diagonal-Long-Range-Order (ODLRO) of the one-particle reduced density matrix for bosons is extended to the two-particle reduced density matrix for fermions and defines naturally the order parameter for superconductivity, to which all the superconductivity effects are associated via the Ginzburg-Landau theory. ODLRO gives also the anomalous factorization property of the two-particle reduced density matrix leading to the generalized Hartree-Fock formulation of the BCS theory.

A macroscopic occupation of a single quantum state follows from ODLRO provided the fermions form bound pairs each extending over a finite coherence distance ξ_0 . The critical temperature is then given by

$$k_B T_c \simeq \Delta_0 \simeq \hbar v_F \xi_0^{-1} \simeq \frac{E_F}{k_F \xi_0} \quad (1)$$

where Δ_0 is the (zero-temperature) superconductivity gap and v_F is the Fermi velocity. In ordinary superconductors the critical temperature is reduced from the degeneracy Fermi temperature ($T_F = E_F/k_B \simeq \hbar^2 n^{2/d} / (m^* k_B) \simeq 10^4 K$) to a much smaller value of the order of 10K by the large ratio between the pair size ξ_0 (of the order of $10^4 A$) and the average distance between Fermi particles in the normal phase ($\simeq 2\pi/k_F$).

The ordinary superconductors provide an example of a natural compromise between the tendency to form local tightly bound pairs (thereby increasing the critical temperature towards the one of preformed boson condensation) and the necessity to extend the size of the pairs to avoid strong fluctuations, which, together with a large effective mass m^* , would drastically decrease the critical temperature.

In the high temperature superconductors [1] T_c from Eq.(1) is of the correct order of magnitude because although the Fermi energy is reduced by an order of magnitude [2], the coherence distance ξ_0 is strongly reduced ($\xi_0 \simeq 10 - 20 A$, $k_F \xi_0 \simeq 10$). However, there is general consensus that in the high temperature superconductors the CuO_2 planes are the prominent structural constituents. This quasi two-dimensionality favors the effects of fluctuations, which tend to destroy the ODLRO. In addition the coherence distance is so short that, because of fluctuations, the range of applicability of the simple BCS mean field theory should be taken with care, whatever the pairing mechanism may be.

On the other hand, the high value of the critical temperature, being incompatible with a large effective mass m^* (experimentally $m^* \simeq 2 - 10 m_0$), makes any explanation based on tightly-bound real space pairs of bipolaron type very unpalatable even though it appears more and more that phonons can not be fully excluded from the game.

In this intermediate situation ($k_F \xi_0 \simeq 10$) between the two previous categories of superfluidity the question arises whether we need a completely new theory, or is it enough to reconsider the BCS theory or its Eliashberg extension, possibly with new pairing mediators and an appropriate symmetry of the order parameter (s- or d-wave pairing). In this latter case a full inclusion of thermodynamic fluctuations only near the transition would be required for a proper description of the behavior of a system belonging to a two component order parameter universality class. However, due to the smallness of ξ_0 the fluctuations should also be relevant far away from the critical temperature [3]. If they are not relevant, as the validity of Eq.(1) seems to imply, an important open issue is to understand the mechanism restricting the fluctuations in these quasi two-dimensional systems.

The difficulty in handling the superconductive phase has a similar counterpart in the normal phase. Usually in the normal phase the high energy processes are eliminated to form the Landau picture of the normal Fermi liquid as a gas of fermionic quasiparticles. A small residual interaction for states around the Fermi level leads to a superconductive instability, which can be handled with a mean-field approximation. This simple representation does not work in the high temperature superconductors due to the presence of various comparable energy scales of different nature. In fact electron spectroscopy in the copper oxides has shown that the systems with one hole per unit CuO_2 cell are charge-transfer insulators with the holes mostly residing in the $3d_{x^2-y^2}$ orbitals of the copper atoms. Additional holes go instead into states with large amplitude on the oxygen planar $2p$ orbitals. The system can then be conveniently described by a three band Hubbard model, which contains the large U_{dd} repulsion on the same Cu site, the strong $p-d$ covalency between copper and the planar oxygen and the Charge-Transfer (CT) energy difference between the effective Cu and

O atomic levels. At this point we can ask ourselves if this strongly correlated quasi two-dimensional fermion system is incompatible with a normal Fermi liquid picture, even though photoemission explicitly indicates the existence of a large Fermi surface satisfying the Luttinger theorem. Many physical quantities, like the in-plane resistivity, indeed deviate from the behaviour predicted by the Landau theory: The antiferromagnetic insulating behavior at and close to half-filling turns upon doping into a strange metal, which at optimal doping displays a linear T-dependence of the in-plane resistivity in the normal phase. Magnetic correlations with a possible spin gap are present in the metallic state in the underdoped regime. At still higher doping the strange metal gradually turns into a normal metal with strongly reduced magnetic correlations. No sharp change in the metallic behavior is experimentally observed by varying the charge carriers or by lowering the temperature. The absence of a clear experimental indication of a transition to a new state for the normal phase, (which could otherwise suggest the form of the symmetry of this anomalous state) and, on the theoretical side, the stability of the normal liquid in standard perturbation theory in 2d as in 3d, make the search for a new metallic phase very hard.

In this context much interest has been devoted to anomalous phases appearing in one-dimensional systems. Due to the close AF phase at low doping and the persistence of AF correlations well inside the metallic phase, Anderson proposed [4], [5] to extend to 2d systems the Resonating Valence Bond (RVB) form of the wavefunction, which gives the solution of the Heisenberg model in 1d in terms of a combination of spin singlets. Peculiar to this solution is the charge and spin decoupling in the excitations. The hypothesis behind this approach [5] is that, away from half-filling, the solution is never a Fermi liquid. In 2d, doping the interacting fermions should lead to a new metallic phase similar to the Luttinger metal occurring in 1d. In this latter metallic phase there is no discontinuity of the occupation number at the Fermi level, but an algebraic singularity, with a non universal exponent. This singularity still defines a Fermi surface satisfying the Luttinger theorem. The marginal Fermi liquid [6], proposed as a phenomenological theory of the normal phase of the cuprates, corresponds to a particular case for which the discontinuity at the Fermi surface goes to zero as the inverse of the logarithm of $|k - k_F|$ rather than algebraically. In the Luttinger liquid the single quasiparticle excitations do not exist at the Fermi surface and the spectrum is made of collective excitations with separate charge and spin modes. The thermodynamic quantities, instead, like specific heat, compressibility, and spin susceptibility, associated with specific limits of the response functions, are those proper of a stable metal. The singularities leading to the anomalous behavior of the single particle properties and to the charge and spin separation must therefore undergo very delicate cancellations in these thermodynamical quantities in order to give rise to a stable metallic phase. Conservation laws, peculiar to 1d, where the Fermi surface is reduced to two points ($\pm k_F$) and the related Ward identities [7], accomplish this task.

An analogous conservation law is valid approximately in $1 < d < 2$, with an increasing accuracy as the Fermi surface is approached. This allows one to sum to all orders in the coupling the relevant small momentum transfer processes leading to the Luttinger liquid in 1d. In this way it is shown that the Luttinger liquid behavior crosses over into a Fermi liquid one as soon as $d > 1$ [8], even though the inverse lifetime of the quasiparticles scales as $|k - k_F|^d$ instead of the square law valid for $d \geq 2$. A breakdown of the Fermi liquid is therefore not obtained in a one band model with short range interactions. As soon as

$d > 1$ the Fermi liquid is a very stable phase: additional degrees of freedom or singular non-perturbative phenomena leading to singular interactions are necessary but not sufficient requirements to obtain a different metallic phase.

It seems to us that these results indicate some difficulties inherent in all models for superconductivity, where pairing arises from a normal phase displaying charge and spin separation in the CuO_2 planes [9].

Many other proposals which could possibly lead to non-Fermi liquid behavior have been left out of this short analysis, e.g. gauge field theories in 2d and the multichannel Kondo (lattice) model. In any case we feel that to settle the question of non-Fermi liquid behavior in 2d has intrinsic difficulties. It is therefore worthwhile to pursue another route, which has a generic validity and makes no drastic assumptions on the normal phase to start with.

The richness of the phase diagram of the high temperature superconducting compounds is a clear indication of the presence of various competing energy terms of the same order of magnitude. As we have already stressed, these terms, on the one hand, make it difficult to handle the different problems separately (like antiferromagnetism, transport in the normal phase and superconductive pairing). On the other hand, in each region of doping and temperature these competing energy terms will favor a tendency towards Phase Separation (PS) [10], a phenomenon which we will discuss extensively in the rest of the paper.

Section II is devoted to the presentation of the PS problem. In Section III PS will be discussed in the framework of an extended three band t-J model. A discussion of the physical implications of the results will be given in Section IV together with our concluding remarks.

II. PHASE SEPARATION: A RELEVANT ISSUE

While on the one hand the solution of the Fermi-liquid vs non-Fermi-liquid dilemma is an intriguing issue, which still deserves intensive investigation, on the other hand the analysis summarized in the previous section clearly indicates that a non-Fermi liquid state is not easily realized in more than one dimension. Therefore it is surely appropriate to investigate different possibilities in order to account for the peculiar normal and superconducting properties of the copper oxides. The general tendency has been the investigation of the various possible scattering mechanisms taking place in the CuO_2 planes. In this latter context, besides the mechanisms involving the presence of (strong) van Hove singularities in the band structure of these oxides [11], an enormous variety of proposals has been put forward, ranging from an enhancement of the q-dependent scattering due to the nesting of the Fermi surface [12], to the scattering with magnetic excitations, both traditional like paramagnons [13] or "exotic", like chiral gauge field fluctuations [14]. Phonons [15] and excitons [16] have also been proposed, witnessing how open (and unfortunately confused) the situation still is. As already stressed, in this situation the need of general unifying paradigms, which are capable of accounting for most properties of the real materials without making too specific assumptions is particularly compelling. In the rest of this paper we will specifically focus on PS [10], which both experimentally and theoretically seems to satisfy this general prerequisite, so that, in the last two years it has become a relevant issue in the context of high T_c superconductivity.

First of all there has been uncontroversial experimental evidence that PS occurs in some high T_c systems. In particular this phenomenon takes place in superoxygenated $\text{La}_2\text{CuO}_{4+x}$

[17] whereas its occurrence has been suggested but not confirmed in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ [17] and in $\text{ErBa}_2\text{Cu}_3\text{O}_{8+x}$ [18]. A different but maybe related phenomenon is the superstructure formation in Bi 2212 and 2232 compounds [19]. Therefore some kinds of inhomogeneities surely occur in most high temperature superconducting materials. The electronic origin of the phenomena is uncertain, though photoinduced conductivity experiments [20] and NMR studies of local structure in metallic $\text{La}_2\text{CuO}_{4+x}$ [21] strongly suggest that the holes due to photodoping or to chemical doping tend by themselves to separate.

PS is also appealing from the theoretical point of view. In fact, whereas the possibility of PS in the Hubbard model was hypothesized some time ago [22], its occurrence has recently been found in the t-J model using a large-N expansion [23] and exact diagonalizations of small clusters [24]. This stimulated the theoretical investigation of the instabilities of purely electronic models. Since then it was found that PS seems to be the rule rather than the exception in the context of models with strongly interacting electrons in the absence of long range Coulomb forces. In fact a slave boson analysis of various models has revealed the occurrence of PS in some parameter region both in models with magnetic interactions like the single band t-J model [25], the three band t-J model [26], [27] and the Kondo-lattice model [28], as well as in models with nearest neighbor Coulombic repulsion [29], [30]. A common feature of these models is the presence of strong correlations between electrons, as reviewed in Ref. [31]. These correlations lead to a substantial reduction of the quasiparticle kinetic energy. As a consequence the stabilizing effect of the kinetic energy, which would lead to the formation of extended uniformly distributed electronic states, is depressed, opening the way to the localizing effects of the short range interactions. This fact is made apparent in those multiband models [26], [29], [30], where it is possible to observe the beginning of PS in the phase diagram region close to the metal-insulator transition. It is in this low doping region where the strong correlations most effectively depress the stabilizing effect of the particle motion and favor the particle segregation.

The analysis of these models, both with magnetic and with nearest neighbor (nn) Coulombic repulsion has revealed suggestive connections between PS and superconductivity. In particular it was found in the context of the infinite-U three-band extended Hubbard model (in this case the short range interaction is due to nn copper-oxygen hole repulsion) [29] that a Cooper instability takes place in the parameter region where the system is a stable Fermi liquid, but close to the line where the compressibility κ diverges. Superconductivity then appears as a kind of precursor effect of PS (at least to leading order in the large-N expansion).

A second PS-superconductivity connection was found [28] in the Kondo-lattice model (here the short range interaction is of magnetic nature), where a mean field analysis indicated that pair formation gives rise to a state with lower energy than the separated phase, showing that the occurrence of superconductivity can stabilize the system preventing PS. This indicates that superconductivity is not necessarily spoiled by PS, as it was implicitly assumed when PS was first presented as a drawback of the one-band t-J model [24]. On the contrary, tendency to PS may favor the pairing formation [28], [29]. Of course the experimental observation of such a phenomenon is strictly related to the diffusional dynamics of charged ions in the systems. This subject has been the object of intensive and interesting experimental investigation [32].

All these phenomena naturally occur in models without a long range Coulomb repul-

sion, which would otherwise prevent the segregation of thermodynamically large clusters of charged particles. Nevertheless dynamical slow density fluctuations can surely survive the presence of Coulomb long range repulsion [33]. This latter interaction is, in fact, most effective at small q's where it prevents the divergence of the static compressibility κ , but not necessarily the dynamical charge susceptibility, which may be large at finite (short) distances (finite large q's).

The presence of long range interactions could explain why copper oxides only rarely display a thermodynamic PS. In particular PS would only be allowed in those systems where a high mobility of oxygen negative ions is present. In this case the negative ions could follow the positively charged holes compensating for the charge unbalance, thereby making Coulomb repulsion ineffective. In this respect superoxygenated La cuprates and 123 compounds are obvious candidates for the observation of a static thermodynamical PS of electronic origin. On the other hand the presence of common structural elements like the CuO_2 planes suggests that the tendency of an electronic PS should also be present in those high T_c materials where it is not observed, due to the presence of long range Coulomb forces, which are not suppressed by the mobility of the negative ions.

From the theoretical point of view the presence of long range Coulomb forces opens the way to many interesting possibilities. On the one hand it has been suggested [33] that low frequency charge density fluctuations could be modelled by means of pseudospin variables thereby introducing a "mesoscopic" description of the system, which is claimed to lead to a mapping into a two-channel Kondo model. This latter model seems to have a similar behavior to the normal properties of the superconducting cuprates. This suggests the possibility [33] that the unusual normal state properties of these systems arise from the scattering of the carriers from soft density modes.

On the other hand the introduction of long range Coulomb forces further enriches the possibilities of fully microscopic models. We mentioned above the existence of the Cooper instability in the proximity of the infinite-compressibility ($\kappa = \infty$) line in the extended infinite-U three band Hubbard model. However, the Maxwell construction reduces the accessible (stable) region around the $\kappa = \infty$ line. The introduction of long range interactions would instead eliminate the small-q instabilities thereby making accessible to the system a much larger region. In particular it could happen that only a small region of a static finite-q instability would remain inaccessible, where incommensurate charge density waves would occur [30]. Close to this region strong attractive forces would be present similar to those occurring at small q near the $\kappa = \infty$ line in the neutral hole case. Of course the long-range repulsion tends to oppose attraction. In this case only a full dynamical treatment would answer the question on the subtle q-dependent screening and cancellation between repelling long range forces and attractive forces arising close to the instabilities. Unfortunately such a detailed microscopic treatment involving both the role of Coulomb forces, total density and CT fluctuations is overwhelmingly difficult and does not seem to be viable in the short term.

From the above discussion it should be remembered that i) PS is a common tendency of models with strong local (Hubbard-like) repulsion and additional short range interactions of various nature; ii) this tendency is expected to be present regardless of the actual existence of a static thermodynamic PS, which depends on the existence of mechanisms (e.g. oxygen diffusion) ruling out the action of the long-range Coulomb forces; iii) two main mi-

microscopic mechanisms have so far been found as possible sources of this tendency, namely the magnetic spin-spin interaction and the copper-oxygen nn Coulomb repulsion. Of primary importance is to recognize that, even though this second mechanism also occurs close to the metal-charge-transfer-insulator transition, it acts most effectively in the finite, large doping regime, forming (dynamic or static) regions of high and moderate doping. On the contrary, the magnetic mechanism is more effective at low doping giving rise to half-filled antiferromagnetic insulating regions and moderately doped metallic regions. The two mechanisms seem therefore dominant in different filling regimes. The simultaneous consideration of these two mechanisms provides a natural and unified description of the effects of the various competing energy terms present in these strongly correlated systems, leading to different phases by varying the charge carriers and the temperature.

Then the question naturally arises whether a real system exists, where both mechanisms play a role. In this case a crucial prerequisite is the possibility of doping the system on a wide range, so as to explore the *tendency* to phase separate by means of a magnetic mechanism at low doping and the *tendency* to phase separate at large doping due to the nn Coulombic repulsion. Obvious candidates are the compounds of the 123 class, where the oxygen content can run from O_6 to O_7 . Last but not least these systems display a rather large oxygen mobility which could at least partially counterbalance the effect of the long range Coulomb forces. Far from being necessary to allow the *tendency* to phase separate, this high mobility of the negative ions could facilitate the experimental detection of the "desire" of PS present in the system.

Interestingly enough the existence of a double (possibly dynamical in nature) PS [18] has already been proposed from inelastic neutron scattering experiments performed on $\text{ErBa}_2\text{Cu}_3\text{O}_{6+x}$ [34].

Whereas the electronic origin of this double (dynamical) PS has to be proven, this system is undoubtedly appealing as a possible candidate to see the two, magnetic and nn Coulombic, mechanisms at work, in support of our general presentation. This point of view will be further elucidated by the analysis of a specific model [35] in the next section.

III. A SPECIFIC EXAMPLE

We consider a three band extended t-J model in order to explicitly show the possibility of the two mechanisms discussed in the previous section coexisting in the same model. In particular we stress that we are not interested in distinguishing between the occurrence of a truly thermodynamical static PS or of a PS, which is dynamical in nature. In particular we will not include long range Coulomb interactions in our model, so that the PSs inherently present should not necessarily be regarded as static.

The starting point [35] is represented by the following Hamiltonian for the CuO_2 planes,

$$\begin{aligned} \mathcal{H} = & (\epsilon_p - \mu) \sum_{i,l,\sigma} p_{i+l,\sigma}^\dagger p_{i+l,\sigma} + (\epsilon_d - \mu) \sum_{i,\sigma} d_{i,\sigma}^\dagger d_{i,\sigma} + \\ & + \sum_{i,l,\sigma} [t_{pd}^\dagger d_{i,\sigma}^\dagger p_{i+l,\sigma} + h.c.] + \sum_{i,l,l',\sigma} (t_{pp}'' p_{i+l,\sigma}^\dagger p_{i+l',\sigma} + h.c.) + \\ & + \frac{U_{pp}}{4} \sum_{i,l,\sigma} n_{i+l,\sigma}^p n_{i+l,-\sigma}^p + V \sum_{i,l,\sigma,\sigma'} n_{i,\sigma}^d n_{i+l,\sigma'}^p + \end{aligned}$$

$$+ J \sum_{(ij),\sigma,\sigma'} d_{i,\sigma}^\dagger d_{i,\sigma} d_{j,\sigma'}^\dagger d_{j,\sigma'} + U_{dd} \sum_i n_{i,1}^d n_{i,1}^d \quad (2)$$

where $d_{i,\sigma}^\dagger$ creates a hole with spin σ in the $d_{x^2-y^2}$ orbital on the copper site i , $p_{i+l,\sigma}^\dagger$ ($l = \pm x/2, \pm y/2$) creates instead a hole in the p_x or p_y orbitals on the oxygen site $i+l$ (we take Cu - Cu distance to be unit). The density operators are defined by $n_{i,\sigma}^d = d_{i,\sigma}^\dagger d_{i,\sigma}$ and $n_{i+l,\sigma}^p = p_{i+l,\sigma}^\dagger p_{i+l,\sigma}$.

The Hamiltonian (2) includes the atomic level energies ϵ_p and ϵ_d on oxygen and copper sites respectively, and the hopping integrals $t_{pd}^\dagger = \pm t_{pd}$ between the d and p orbitals and $t_{pp}'' = \pm t_{pp}$ between the p orbitals [36]. This tight-binding part reproduces therefore the p - d covalent nature of the CuO_2 planes. The interaction terms are, instead, represented by the Coulombic interaction V between nn Cu and O holes, by the Cu-Cu superexchange term J and by the Hubbard repulsion U_{dd} between holes on the same copper site. This last interaction is by far the largest energy scale ($U_{dd} \sim 10\text{eV}$) in copper oxides so that the $U_{dd} \rightarrow \infty$ limit was considered by means of a standard slave-boson technique [37].

The above model is particularly suitable to describe the many different behaviors occurring upon doping in the copper oxides. In these systems the antiferromagnetic insulator which is present in the stoichiometric and lightly doped compound turns into the *strange metal* with magnetic correlations, as it was discussed in Section I. At still higher doping the strange metal gradually turns into a normal metal with strongly reduced magnetic correlations. The spin degrees of freedom therefore play a major role at low doping, when charge degrees of freedom are essentially frozen out due to the presence of strong correlations. Charge degrees of freedom become gradually more relevant in the intermediate and high doping regimes. This interplay of strong correlations in different degrees of freedom is well schematized by the above model.

It should be noted that the model in Eq.(2) gives rise to a Cu-Cu superexchange interaction even in the absence of the term proportional to J . However, due to the technical complexity of the model a mean-field approximation was used. Since this approximation neglects the virtual processes leading to the Cu-Cu superexchange interaction, the term proportional to J was explicitly added to keep into account this important piece of physics and the value of this coupling was fixed according to the usually accepted experimental value ($J = 0.1t_{pd}$ with $t_{pd} = 1.3\text{eV}$).

It is worth stressing that the mean field approximation within the slave boson scheme is very different from the conventional Hartree-Fock procedure and, contrary to this latter, is even able to reproduce the Mott-Hubbard charge-transfer insulating character of the CuO_2 planes at half-filling. On the other hand the much weaker interactions V , U_{pp} and J can be safely decoupled via Hartree-Fock factorizations. To investigate the normal and the superconducting phases on equal footing both normal and superconducting decouplings were considered, to which the subscript "1" and "2" were appended respectively.

For the sake of simplicity, the magnetic interaction was treated neglecting that decoupling giving rise to spin long range order. This choice was dictated by the fact that in the real high temperature superconductors antiferromagnetism is rapidly destroyed by doping, so that one can directly focus on a nn singlet decoupling $\Delta_{ij}^1 = (J/2) \sum_\sigma (d_{i,\sigma}^\dagger d_{j,\sigma})$. This latter has been widely used to suitably describe at mean-field level the magnetic correlations present in the metallic phases [38], [39]. Within this scheme the antiferromagnetic insulator is mimicked by the so called dimer phase having the same unit cell doubling, where the parameter Δ_{ij}^1

assumes different values on the bonds pointing in different directions ($\Delta_1^x \neq \Delta_1^y \neq \Delta_1^z$). The magnetically correlated metal is, instead, represented by the uniform phase where all the bonds have the same value ($\Delta_1^x = \Delta_1^y = \Delta_1^z = \Delta_1$). The metallic phase without magnetic correlations is characterized by a vanishingly small value of Δ_1 .

On the other hand, the anomalous order parameter Δ_2 arises as a consequence of the attractive superexchange interaction J and represents the occurrence of a superconducting phase in this mean field approximation [40]. The possible occurrence of s-wave as well as d-wave superconductivity was investigated. This latter was always found to be more stable. Thus, superconducting phases of d-wave type only will be considered in this context.

The numerical solution of the self-consistency equations together with the condition for the chemical potential fixing to $(1 + \delta)$ the number of particles per CuO_2 cell yields the phase diagram of the model for various values of the physical parameters [35].

The $T = 0$ phase diagram is shown in Fig.1. A metal-insulator transition is found at half filling by varying the distance between the atomic levels $\epsilon_p - \epsilon_d$. This transition takes place between a magnetically uniform metal ($\Delta_1 \sim J, \Delta_2 = 0$) and an insulating phase with dimer magnetic symmetry. At low doping the system is unstable due to the presence of the dimer phase (or of the antiferromagnet), which tends to eject doped holes leading the system towards PS. Moreover, when V is sufficiently large, the system is driven towards the charge-transfer (CT) instability at intermediate doping. To our knowledge the CT mechanism is the only one which provides a PS in the intermediate- and high-doping regimes. It must be emphasized that these two mechanisms for phase separation do not exclude each other, but play their role in different regions of doping. The two PS regions merge in the vicinity of the metal-insulator transition.

FIG.1: Phase diagram ($\epsilon_p - \epsilon_d$) vs. the doping δ with $T = 0.002\text{eV}$, $t_{pd} = 1.4\text{eV}$, $t_{pp} = 0.4\text{eV}$, $J = 0.2\text{eV}$, $V = 3.0\text{eV}$ and $U_{pp} = 0.5\text{eV}$. Solid lines indicate the phase transition lines. The shaded area delimited by the dashed lines indicates the phase separation region determined via the Maxwell construction. The diamond

indicates the metal-insulator transition.

A d-wave pairing phase ($\Delta_1, \Delta_2 \sim J$) is stable in the intermediate-doping regime and at large CT gaps, with the correlated metal ($\Delta_1 \sim J, \Delta_2 = 0$) nearby. This latter smoothly crosses over to the uncorrelated metal ($\Delta_1 \simeq 0, \Delta_2 = 0$), which is the stable phase at high doping.

The large overlap between the phase separation region and the magnetically induced superconductivity region strongly suggests that the two phenomena are related. As it was previously recalled, a similar occurrence was found to occur in the Kondo-lattice model [28], where a magnetism mediated attractive force in the particle-hole channel leads to phase separation and, at the same time, makes possible a stable homogeneous superconducting phase. Contrary to the superexchange term J , the nn interaction V , being repulsive, cannot induce pairing in mean field approximation. However, the analyses in Refs. [29] and [30] have shown that attraction can appear close to the CT phase separation instability when CT fluctuations, enhanced by V , are considered. This mechanism therefore extends to higher doping and lower bare CT gaps the superconducting phase shown in the phase diagram of Fig. 1. Moreover, also in this case, superconductivity could stabilize the system with respect to phase separation, thus reducing the phase separation region.

IV. COMPARISON WITH THE EXPERIMENTS

Without pretending a quantitative agreement between the model in Eq.(2) and the real systems, we present some general experimental facts and show that they, not only are not in contrast with, but even find a rather natural explanation, within the two PS scenario.

Specifically the spectra of low energy crystal-field excitations of Er^{3+} in $\text{ErBa}_2\text{Cu}_3\text{O}_{6+x}$ [34], [18] result from the superposition of three distinct stable states. At an oxygen concentration ranging from 6 up to 6.6, the system seems to phase separate between an antiferromagnetic insulating phase and an intermediate-doping metallic phase. Then the AF insulating phase disappears and the peak corresponding to a high-doping metallic phase arises. In the concentration region between $x = 0.6$ and $x = 0.95$ the two metallic states coexist, whereas the pure high-doping metallic phase seems to be present in the overdoped $x \geq 0.95$ phase. It is important to realize that this analysis was carried out with a local dynamical probe and was therefore able to provide information on the tendency to phase separation regardless the actual occurrence of a true long-range thermodynamical segregation of different phases [41].

It should be noted that, if one insists in assuming the electronic origin of both PSs, it is quite difficult to interpret the second PS as being also due to a magnetic mechanism. In fact the large doping makes unlikely the efficiency of magnetism in driving the system into an instability.

The experiments show a small region of doping where the three peaks may simultaneously coexist, indicating that this system may have parameters values in the region of Fig.1, where the two PS are merged. In this case the slow density fluctuations arising from the Coulomb frustrated phase separation can simultaneously occur along two distinct channels according to the two distinct driving mechanisms hypothesized in this paper. A first channel involves density fluctuations between the AF insulator and the intermediate-doping metal mainly

driven by magnetism, whereas the charge-transfer driving force would be responsible for the slow fluctuations between the intermediate-doping metal and the high doping metal. The fluctuating bubbles of the intermediate-doping metal would then be present at various doping concentrations as a result of the overlap between the two merged "phase separations". This second interpretation would account for both the large width of the peak related to the intermediate-doping metal shown in the experiments and the persistence of some magnetic effects at very large doping. In particular it would also naturally explain the presence of broad maxima at $T^* > T_c$ in the in highly doped (up to $x = 0.92$) 123 samples [42]. The (pseudo)-gap in the spin excitations [43] usually advocated to explain this behaviour would then be associated to the finite-size spin-waves in the AF density fluctuations [33] arising from the first fluctuation channel.

Another experimental consequence of this scenario would be the existence of a double signal in the NMR copper spin relaxation rate $(T_1T)^{-1}$ arising from the contemporary presence of the AF insulating phase and the high-doping metallic phase. A first signal would be present due to the fluctuations between the AF insulator and the intermediate-doping metal and would provide the spin-gap maximum at T^* . A second signal would arise from the fluctuations between the intermediate-doping and the high-doping metals and it would display the standard decrease of the relaxation rate at $T_c = 92K$ due to the opening of the superconducting gap. A close inspection of the NMR data seems to support this possibility, but further more detailed experimental investigation is required to make any definite statements.

According to the discussion of Section II, phase separation provides a possible scenario for the developing of an exotic way to induce pairing and, at the same time, an anomalous normal state. The example discussed in Section III indicates that various mechanisms for PS can coexist. In particular, the simultaneous presence of magnetic and CT terms in the Hamiltonian allows for two distinct tendencies towards PS. In turn the two physical mechanisms drive density fluctuations occurring along two distinct channels. The smooth change of the relative weight of these fluctuations of two different types may produce a gradual change with doping of the characteristics of the metal in the normal phase. On the other hand, the attractive forces produced by the tendency to phase separate driven by the combination of the two mechanisms may lead to superconductivity over an extended range of doping.

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