

Two-gap model for underdoped cuprate superconductors

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Various properties of underdoped superconducting cuprates, including the momentum-dependent pseudogap opening, indicate a behavior which is neither BCS- nor Bose-Einstein condensation (BEC)- like. To explain this issue we introduce a two-gap model. This model assumes an anisotropic pairing interaction among two kinds of fermions with small and large Fermi velocities representing the quasiparticles near the M and the nodal points of the Fermi surface, respectively. We find that a gap forms near the M points resulting in incoherent pairing due to strong fluctuations. Instead, the pairing near the nodal points sets in with phase coherence at lower temperature. By tuning the momentum-dependent interaction, the model allows for a continuous evolution from a pure BCS pairing (in the overdoped and optimally doped regime) to a mixed boson-fermion picture (in the strongly underdoped regime).

The underdoped cuprates are characterized by a pseudogap opening below a strong doping (δ) dependent crossover temperature $T^*(\delta)$, above the superconducting critical temperature $T_c(\delta)$.¹ By decreasing the doping, the temperature T^* increases, while the superconducting critical temperature T_c decreases until the insulating state is reached. The different behavior of T^* and T_c as doping is varied, finds a counterpart in the different behavior of the coherence energy scale, obtained in Andreev reflection measurements,² and the single-particle gap, observed both in angle-resolved photoemission (ARPES) and in tunneling experiments.¹ This has triggered a very active debate on the relevance of a non-BCS superconductivity and of a BCS-BEC crossover in these materials.³⁻⁶ In particular, ARPES shows that below T^* the gap opens around the M points of the Brillouin zone [i.e., $(\pm\pi, 0), (0, \pm\pi)$] suggesting that T^* can be interpreted as a mean-field-like temperature where electrons start to form local pairs without phase coherence. However, it is also found⁷ that below T^* , substantial portions of the Fermi surface remain gapless. This behavior can be described neither by BCS nor by Bose-Einstein condensation (BEC) schemes. Instead, it is suggestive of strong pairing between the states around the M points and of weak coupling near the zone diagonals. Various other experiments^{8,9} carried below T_c show a doping and temperature dependence of the gap anisotropy and therefore are again suggestive of a strong anisotropy in the pairing potential.

In this paper we explore a different direction (neither BCS nor BEC) focusing on the consequences of a strongly anisotropic interaction. To this aim we introduce a two-gap model, where strongly paired fermionic states can coexist and interplay with weakly coupled pairs in different regions of the Fermi surface (FS). This line of thinking was partly explored in Refs. 5 and 6, where only the extreme strong-coupling limit of one component was considered. In particular, the view of Ref. 6 would allow only the description of the very underdoped region of the cuprate phase diagram. Our approach, instead, turns out to be sufficiently flexible to investigate with continuity the evolution of the bifurcation (taking

place around optimal doping in the real systems) between a mean-field-like pairing temperature T^* and the coherence superconducting temperature T_c . We implement our model by a two-band system with different intraband and interband pairing interactions. One band has a large Fermi velocity v_F and a small attraction giving rise to largely overlapped Cooper pairs with weak superconducting fluctuations. On the contrary, the other band has a small v_F and a large attraction resulting in tightly bound pairs having strong fluctuations. At variance from the models of mixed fermions and bosons, we keep the fermionic nature of both the weakly and strongly bound Cooper pairs.

A possible realization of a strongly momentum-dependent effective interaction in underdoped cuprates has been proposed in connection to the occurrence of a charge instability for stripe formation.^{10,11} It was indeed suggested that the tendency to spatial charge order (which evolves into a spin-charge stripe phase by lowering the doping) gives rise to an instability line. This line $T_{\text{stripe}}^c(\delta)$ starts from a quantum critical point (QCP) at $T=0$ near optimal doping and increases by lowering the doping. By approaching the instability line the pairing is mediated by the strong attractive quasical stripe fluctuations, which affect the states on the FS in a quite anisotropic way:

$$V_{\text{eff}}(\mathbf{q}, \omega) \approx \tilde{U} - \frac{V}{\kappa^2 + |\mathbf{q} - \mathbf{q}_c|^2 - i\gamma\omega}, \quad (1)$$

where \tilde{U} is the residual repulsive interaction between the quasiparticles, γ is a damping parameter, and \mathbf{q}_c is the wave vector of the stripe instability. The crucial parameter κ^2 is a mass term proportional to the inverse square of the correlation length of charge order ξ_c^{-2} and provides a measure of the distance from criticality. At $T=0$, in the overdoped regime, κ^2 is linear in the doping deviation from the critical concentration $\kappa^2 \propto (\delta - \delta_c)$. On the other hand, in the finite-temperature region above δ_c , $\kappa^2 \propto T$. In the underdoped regime, κ^2 vanishes approaching the instability line $T_{\text{stripe}}^c(\delta)$

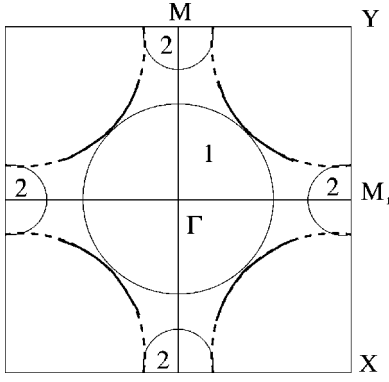


FIG. 1. Sketch of the Fermi surface of underdoped cuprates with quasiparticle arcs (thick solid line), and patches of quasilocalized states (thick dotted line), and the Fermi surface of the two-band spectrum (thin solid line).

and extends the singular potential to finite temperatures. For $\kappa^2 \approx 0$, the fermionic states around the M points are such that $\mathbf{k}_F - \mathbf{k}'_F \sim \mathbf{q}_c$ and interact strongly. These are the so-called “hot spots,”¹² they have a low dispersion, and possibly form tightly bound local pairs giving rise to the pseudogaps below $T^* \approx T_{\text{stripe}}^c(\delta)$. On the other hand, “cold” states in the arcs of FS around the zone diagonals $\Gamma - Y$ or $\Gamma - X$ (nodal points) have larger dispersions and interact more weakly since V_{eff} is now cut off by \mathbf{q}_c . In the underdoped regime, $\kappa^2 \approx 0$ at higher and higher temperatures by lowering the doping and V_{eff} has a more dramatic effect. On the contrary, in going to the optimum and the overdoped region V_{eff} is cut off first by the temperature and then by the doping itself. All the states then interact more isotropically.

The two-gap model. Irrespective of the origin of the anisotropy, in the presence of a strong momentum dependence both of (i) the effective pairing interaction and (ii) the Fermi velocity, we must allow for enough freedom of the pairing and of its fluctuations in order to capture the relevant physical effects of the anisotropy. Following the above discussion we introduce a simple two-band model for the cuprates. We describe the quasiparticle arcs of FS about the nodal points by a free electron band (labeled below by the index 1) with a large Fermi velocity $v_{F1} = k_{F1}/m_1$ and the hot states about the M points with a second free electron band, displaced in momentum and in energy from the first, with a small $v_{F2} = k_{F2}/m_2$ (see Fig. 1).

The assumed electronic spectrum consists therefore of two different free electron dispersions, $\epsilon_1(\mathbf{p}) = |\mathbf{p}|^2/2m_1$ and $\epsilon_2(\mathbf{p}) = |\mathbf{p} - \mathbf{p}_0|^2/2m_2 + \epsilon_0$, displaced by a momentum \mathbf{p}_0 and by an energy $\epsilon_0 \sim E_{F1}$ introduced to allow the chemical potential to cross both bands: $E_{F1} = \epsilon_0 + E_{F2}$. To connect our two-band structure with the single-band dispersion of the cuprates, we choose $\mathbf{p}_0 = (\pm\pi, 0), (0, \pm\pi)$.

This choice gives rise to two branches for band 2 along the x and y directions. Moreover, we only consider Cooper pairs of zero total momentum formed by time-reversed momentum eigenstates. Therefore, the 2-2 pairs are always formed by $(\mathbf{k}, -\mathbf{k})$ states on portions of band 2, symmetrically located on opposite sides with respect to the $\Gamma \equiv (0, 0)$ point. If the pairs have a s -wave symmetry, the branches along x and y of band 2 are equivalent and just one can be considered. On the other hand, in the case of d -wave pairing,

the pairs in the branch along x have a different phase from the pairs in the branch along y and both branches have to be treated. Since in this paper our main interest is the interplay between strongly and weakly coupled pairs irrespective of their symmetry, for simplicity we consider the s -wave problem. The model Hamiltonian for pairing in the two-band system is taken to be

$$H = \sum_{k\sigma i} \epsilon_{ki} n_{k\sigma i} + \sum_{kk'p i j} V_{ij}(k, k') c_{k'+p \uparrow j}^\dagger c_{-k' \downarrow j}^\dagger c_{-k \downarrow i} c_{k+p \uparrow i}, \quad (2)$$

where i and j run over the band indices 1 and 2 and σ is the spin index. The interaction is approximated by a BCS-like attraction given by

$$V_{ij}(k, k') = -g_{ij} \Theta(\omega_0 - |\xi_i(k)|) \Theta(\omega_0 - |\xi_j(k')|), \quad (3)$$

with an energy cutoff ω_0 . The strongly q -dependent effective interaction in the particle-particle channel $V_{\text{eff}}(\mathbf{q} = \mathbf{k} - \mathbf{k}')$ of the original single-band system is accounted for by the 2×2 scattering matrix \hat{g} . The matrix elements g_{ij} couple the electrons within the same band (g_{11} and g_{22}) and between different bands ($g_{12} = g_{21}$). The self-consistency equation for the superconducting fluctuation propagator¹³ in the matrix form is given by $\hat{L} = \hat{g} + \hat{g} \hat{\Pi} \hat{L}$, where the particle-particle bubble operator for the two-band spectrum has a diagonal 2×2 matrix form with elements $\Pi_{11}(q)$ and $\Pi_{22}(q)$.¹⁴ The resulting fluctuation propagator is given by

$$\hat{L}(q) = \begin{pmatrix} \tilde{g}_{11} - \Pi_{11}(q) & \tilde{g}_{12} \\ \tilde{g}_{12} & \tilde{g}_{22} - \Pi_{22}(q) \end{pmatrix}^{-1}; \quad (4)$$

where we have defined $\tilde{g}_{ij} \equiv (\hat{g}^{-1})_{ij}$. It turns out to be useful to define the temperatures T_{c1}^0 and T_{c2}^0 as $\tilde{g}_{11} - \Pi_{11}(0, T) = \tilde{g}_{11} - \rho_1 \ln(\omega_0/T) \equiv \rho_1 \ln(T/T_{c1}^0)$, $\tilde{g}_{22} - \Pi_{22}(0, T) = \tilde{g}_{22} - \rho_2 \ln(\omega_0/T) \equiv \rho_2 \ln(T/T_{c2}^0)$, where $\rho_i = m_i/(2\pi)$ is the density of states of the i th band. In the underdoped regime, to emulate the hot and cold points related, for instance, to the system near a stripe instability, we assume the following relations between the g_{ij} elements: $g_{22} \approx V/\kappa^2 \gg g_{11} \approx V/|\mathbf{q}_c|^2 \approx g_{12}$. Then, one has $\tilde{g}_{11} \approx 1/g_{11}$, $\tilde{g}_{22} \approx 1/g_{22}$, $\tilde{g}_{12} \approx -g_{12}/(g_{11}g_{22})$. In this limit, T_{c1}^0 and T_{c2}^0 (with $T_{c2}^0 \gg T_{c1}^0$) assume the value of the two BCS critical temperatures for the two decoupled bands. The mean-field BCS superconducting critical temperature for the coupled system T_c^0 is defined by the equation $\det \hat{L}^{-1}(\mathbf{q}=0, T_c^0) = 0$. We obtain $T_c^0 > T_{c2}^0$, given by

$$T_c^0 = \sqrt{T_{c1}^0 T_{c2}^0} \exp \left[\frac{1}{2} \sqrt{\ln^2 \left(\frac{T_{c2}^0}{T_{c1}^0} \right) + \frac{4\tilde{g}_{12}^2}{\rho_1 \rho_2}} \right]. \quad (5)$$

The Ginzburg-Landau approach. The role of fluctuations can be investigated within a standard Ginzburg-Landau (GL) scheme, when both $\rho_2 g_{22} \omega_0 < E_{F2}$ and $\omega_0 < E_{F2}$. Under these conditions the chemical potential is not affected significantly by pairing. Moreover, in order to remain within the GL approach, we will assume that fluctuations from the BCS result are not too strong. The relevance of the space fluctuations of the order parameter is assessed by the gradient term coefficient η , which provides the momentum dependence of

the fluctuation propagator in Eq. (4). In particular, the expansion of the particle-particle bubbles, in terms of q , reads $\Pi_{11}(q) \approx \Pi_{11}(0) - \rho_1 \eta_1 q^2$ and $\Pi_{22}(q) \approx \Pi_{22}(0) - \rho_2 \eta_2 q^2$. Here η_i ($i=1,2$) is the gradient term coefficient of the i th band width, in 2D and for a free electron band, is given by $\eta_i = (7\zeta(3)/32\pi^2)v_{Fi}^2/T^2$, with $\eta_1 \gg \eta_2$.¹⁵ In the absence of the interband coupling g_{12} , η_1 provides the (large) gradient term coefficient corresponding to (the weak) superconducting fluctuations for the band with a large v_{F1} , while (the small) η_2 corresponds to (strong) superconducting fluctuations for band 2. For the coupled system near T_c^0 , the coefficient η in terms of η_1 and η_2 is obtained by evaluating $(\hat{L}^{-1})_{ij} \propto (\epsilon + \eta q^2)$ in terms of the relative temperature deviation $\epsilon \equiv (T - T_c^0)/T_c^0$. We get the expression

$$\eta = \frac{\rho_1(\tilde{g}_{22} - \Pi_{22})\eta_1 + \rho_2(\tilde{g}_{11} - \Pi_{11})\eta_2}{-T(\tilde{g}_{22} - \Pi_{22})d\Pi_{11}/dT - T(\tilde{g}_{11} - \Pi_{11})d\Pi_{22}/dT}, \quad (6)$$

where all the bubbles are evaluated at $q=0$. Using the definitions for $T_{c1,2}^0$ and the condition $\det \hat{L}^{-1}(\mathbf{q}=0, T_c^0) = 0$, the coefficient η can be explicitly written as

$$\eta = \alpha_1 \eta_1 + \alpha_2 \eta_2, \quad \text{with} \quad \frac{\alpha_1}{\alpha_2} = \frac{\tilde{g}_{12}^2}{\rho_1 \rho_2 \ln^2(T_c^0/T_{c1}^0)}, \quad (7)$$

and $\alpha_1 + \alpha_2 = 1$. The presence of a fraction of electrons with a large η_1 increases the stiffness of the whole electronic system (i.e., increases η with respect to η_2). However, when the mean-field critical temperature T_c^0 is much larger than T_{c1}^0 the correction to η_2 due to the interband coupling is small. At the same time, the Ginzburg number is large enough to imply a sizable mass correction $\delta\epsilon(T)$ to the ‘‘mass’’ $\epsilon(T)$ of the bare propagator $\hat{L}(q)$. The renormalized critical temperature T_c^r , given by the equation $\epsilon(T_c^r) + \delta\epsilon(T_c^r) = 0$, is lower than T_c^0 .¹⁶ By evaluating the renormalized gradient term coefficient η^r in the presence of the mass correction, we find that this is still given by Eq. (7) with T_c^0 replaced by T_c^r . Therefore, $\eta^r = \eta(T_c^r)$ is greater than $\eta(T_c^0)$. This result indicates that the mass renormalizations of the fluctuation propagator tends to lower T_c and, at the same time, increases the gradient term coefficient η by increasing the coupling to η_1 . As a consequence, the effective Ginzburg number is reduced and the system is stabilized with respect to fluctuations, allowing for a coherent superconducting phase even in the limit $\eta_2 \rightarrow 0$. Within the GL approach, we associate the temperature $T_c^0 \sim T_{c2}^0$ to the crossover temperature T^* and T_c^r to the superconducting critical temperature T_c of the whole system. In the region $T_c < T^*$, the pseudogap is formed in band 2. Superconducting fluctuations only affect band 2 while they are immaterial for band 1, where the Fermi surface is maintained until phase coherence sets in. Within the stripe-QCP scenario, the coupling g_{22} is related to the singular part of the effective interaction mediated by the stripe fluctuations. g_{22} is the most doping dependent coupling and attains its largest value in the underdoped regime, where κ^2 vanishes at higher temperatures. The regular parts of the interaction g_{11} and g_{12} , being cut off by \mathbf{q}_c , are instead only weakly doping dependent. In

the region of validity of the GL approach, the explicit calculations show that $r(\delta) \equiv (T_c^0 - T_c^r)/T_c^0 \approx (T^* - T_c)/T^*$ is increasing by increasing g_{22} , i.e., by decreasing doping. For small values of r , we find that both T^* and T_c increase. This regime corresponds to the overdoped and optimally doped region. Specifically, above optimum doping, g_{22} and g_{11} become comparable and the two lines merge together. For $r \sim 0.25 \div 0.5$, T_c is instead decreasing while T^* is always increasing by decreasing doping. The large values of r , which are attained in the underdoped region, show that we are reaching the limit of validity of our GL approach. We think, however, that the behavior of the bifurcation between T^* and T_c represents correctly the physics of the pseudogap phase, while a quantitative description would require a more sophisticated approach such as a RG analysis.

The strong-coupling limit. In the very low doping regime, where T^* has increased strongly, the value of g_{22} can be so large to drive the system in a strong coupling regime for the fermions in band 2 ($\rho_2 g_{22} \omega_0 > E_{F2}$). In this case, taking $\omega_0 > E_{F2}$, the chemical potential is pulled below the bottom of band 2. In this limit of tightly bound 2-2 pairs, the propagator of the superconducting fluctuations in band 2, i.e., $L_{22}(q)$, assumes the form of a single pole for a bosonic particle. Since E_{F1} is still the largest energy scale in the problem, the fermionic character of the particles in band 1 is preserved. The critical temperature of the system is again obtained by the vanishing of $\det \hat{L}^{-1}(q=0)$ where, however, the chemical potential is now self-consistently evaluated including the self-energy corrections to the Green function in band 2 and the fermions left in band 1. One gets $\Pi_{22} = \rho_2 \omega_0 / |\mu_2|$ and

$$T_c^0 = T_{c1}^0 \exp \left[\frac{\tilde{g}_{12}^2}{\rho_1 \rho_2 \omega_0} \frac{|\mu_2| |\mu_B|}{(|\mu_2| - |\mu_B|)} \right], \quad (8)$$

where μ_2 is the chemical potential measured with respect to the bottom of band 2 and $|\mu_B| = \rho_2 g_{22} \omega_0$ represents the bound-state energy. The calculation of Π_{22} at small q leads to a finite value of $\eta_2 = 1/(8m_2 |\mu_2|)$, while the small- q expansion of $\det \hat{L}^{-1}$ provides the new η coefficient¹⁷

$$\eta = \eta_1 + \rho_1 \rho_2 \omega_0 \frac{g_{22}^2}{|\mu_2|} \ln^2(T_c^0/T_{c1}^0) \eta_2. \quad (9)$$

In this strong-coupling case, most of the non-mean-field effect has been taken into account by the formation of the bound state occurring at a very high temperature of the order $\rho_2 g_{22} \omega_0$, which provides the new T^* in this regime. $\eta \sim \eta_1$ stays sizable and the fluctuations will not strongly further reduce T_c^r with respect to T_c^0 : $T_c \approx T_c^r \approx T_c^0$. In this low-doping regime $(T^* - T_c)/T^*$ approaches its largest values before T_c vanishes.

The strong coupling limit of our model shares some similarities as well as some important differences with phenomenological models of interacting bosons and fermions.^{5,6} In particular, in the model of Ref. 6, pairs of noninteracting electrons are scattered from the Brillouin zone near the nodal points into dispersionless boson states, localized about the M points at an energy ϵ_B . The correspondence with our model can be seen by noticing that the tightly bound bosonic states

correspond to $\rho_2 g_{22} \omega_0 \gg E_{F2}$ and $g_{11} = 0$. The tightly bound dispersionless bosonic states are fully incoherent ($\eta_2 = 0$), while the fermionic states are unpaired as long as bosons and fermions are independent. The fermion-boson coupling g_{12} effectively introduces an e - e coupling of the order of $\rho_1 \rho_2 \omega_0 g_{12}^2 / \epsilon_B$ and drives the system to superconductivity. In this particular limiting case of our model, we recover the results of Ref. 6 with an explicit expression for the bosonic level $\epsilon_B = |\mu| - |\mu_B|$, while in Ref. 6 it is a free phenomenological parameter.

Conclusions. In our paper we have analyzed the pairing properties of the underdoped cuprates in terms of an effective two-gap model, motivated by the strong anisotropy of the band dispersion and of the effecting pairing interaction. The crucial schematization was based on the introduction of two bands weakly coupled in order to preserve a substantial distinction between the superconducting order parameter in different regions of the momentum space. This has to be contrasted with more standard approaches producing one

single gap (even with complicated momentum dependence) and a common fluctuating order parameter all over the FS. Our approach allows for different fluctuation regimes for pairs in different \mathbf{k} regions. According to our analysis, the strongly bound pairs forming at high temperature T^* can experience large fluctuations until the system is stabilized by the coupling with less bound BCS-like states, leading to a coherent superconducting state at $T_c < T^*$. T_c and T^* merge around or above optimum doping, where g_{22} , according to our stripe scenario, becomes of the order of g_{11} . Our model shares similarities with the fermion-boson models for cuprates^{5,6} to which it reduces in the strong-coupling limit for $g_{22} \gg g_{11} \approx 0$. The two-gap model considered here applies to a much wider doping region and is more suitable to describe the crossover to the optimal and over-doped regime, where no preformed bound states are present and the superconducting transition is quite similar to a standard BCS transition.

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¹⁴Since the model only considers pairing between time-reversed states with zero total momentum, fermionic particle-particle bubbles involving one fermion on band 1 and one fermion on band 2 never appear in the ladder resummation for the propagator $\hat{L}(q)$.

¹⁵In the superconducting cuprates ARPES [see, e.g., D. S. Marshall *et al.*, Phys. Rev. Lett. **76**, 4841 (1996) and J. C. Campuzano *et al.*, Phys. Rev. B **53**, R14 737 (1996)] indicates that $v_{F1}/v_{F2} \sim 3$, so that $\eta_1/\eta_2 \sim 10$.

¹⁶In the explicit calculation we assume that the largest contribution to $\delta\epsilon(T)$ comes from the first order self-energy corrections to the bare Green functions of the p - p bubbles of Eq. (4). In these corrections, we cut off the 2D logarithmic divergencies by a small interlayer coupling.

¹⁷Neglecting the temperature dependence of Π_{22} in Eq. (6) and using Eq. (8), one can show that, despite the different physical situation, this strong-coupling form of η assumes the same expression as in Eq. (7).