d-wave superconductivity near charge instabilities

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(Received 30 May 1996)

We investigate the symmetry of the superconducting order parameter in the proximity of a phase separation or of an incommensurate charge-density-wave instability. The attractive effective interaction at small or intermediate transferred momenta is singular near the instability. This strongly q-dependent interaction, together with a residual local repulsion between the quasiparticles and an enhanced density of states for band structures appropriate for the high-temperature superconducting oxides, strongly favors the formation of d-wave superconductivity. The relative stability with respect to superconductivity in the s-wave channel is discussed in detail, finding this latter hardly realized in the above conditions. The superconducting temperature is mostly determined by the closeness to the quantum critical point associated with the charge instability and displays a stronger dependence on doping with respect to a simple proximity to a van Hove singularity. The relevance of this scenario and the generic agreement of the resulting phase diagram with the properties displayed by high-temperature superconducting oxides is discussed. [S0163-1829(96)02645-8]

I. INTRODUCTION

An increasing complexity in the structure of the order parameter of the high- T_c superconductors is coming out from the experiments. Strongly anisotropic behavior in Bi₂Sr₂CaCu₂O_{8+ δ} (BiSCCO) materials is evident from photoemission experiments. A very small value of the gap is measured along the ΓY direction ($|k_x| = |k_y|$) compatible with a line of nodes according to the *d*-wave pairing.^{1,2} Evidence for *d*-wave pairing comes also from penetration depth measurements and from several Josephson-coupling experiments mostly in YBa₂Cu₃O_{7- δ} (YBCO).³ Phase-sensitive experiments, however, in some cases also provide evidence for *s*-wave pairing.⁴ In this context it is worth considering the implications as well as the various possible origins of superconducting order parameters of different symmetries.

In this paper we analyze the symmetry (d wave vs swave) and the doping dependence of the critical temperature T_c for the pairing interactions which arise near a charge instability. Specifically, we will show that a *d*-wave pairing comes out in a region of the phase diagram near a phase separation (PS) or an incommensurate charge-density-wave (CDW) instability. The latter situation arises in strongly correlated systems when Coulomb forces forbid a thermodynamic PS, giving rise to a density instability at a specific finite wave vector q_{CDW} . In a recent Letter it was shown that near these charge instabilities a singular scattering among quasiparticles arises which may be responsible for the anomalous behavior of the normal phase above T_c .⁵ According to our analysis, the same singular scattering may provide the strong pairing mechanism needed for high- T_c cuprate superconductors. The order parameter turns out to be strongly anisotropic and, under quite general conditions, of *d*-wave symmetry. This happens in the proximity of both PS and CDW's. In addition, the analysis of the CDW case reveals an interesting interplay between the finite-momentum instability and the geometry of the Fermi surface, leading to the appearance of specific structures in the superconducting gap. Finally, by considering the PS and CDW instabilities at zero temperature within the context of quantum transitions, we will argue on a possible mechanism for the existence of both strong variations and plateaus in the dependence of the superconducting critical temperature on doping. We shall also comment on the relevance of CDW's in providing a consistent scenario for both optimal doped and underdoped cuprate materials.

II. PROXIMITY TO PS

The origin of *d*-wave pairing is usually attributed to the relevance of electron-electron (e-e) scattering at large wave vector, specifically at $\vec{q} \equiv (\pi, \pi)$ due to strong antiferromagnetic spin fluctuations.^{6,7} Alternatively, charge fluctuations near a PS (in particular driven by excitonic effects in a threeband extended Hubbard model) have already been proposed as a source of *d*-wave pairing.^{8–10} Here we shall exploit the general feature that an effective interaction with on-site repulsion and singular attraction⁵ at small *q* is generated nearby a PS, regardless of the forces driving the instability.^{8–13}

An effective e - e interaction with attraction at small q and weak on-site repulsion was already advocated to explain the strong anisotropy in the gap observed in angle-resolved photoemission spectroscopy (ARPES) experiments.¹⁴⁻¹⁶ In these analyses the anisotropy of the gap (of *s*-wave symmetry) is driven by the anisotropy of the density of states due to momentum decoupling induced by the small q scattering, which for a given point k in momentum space couples only nearby states. Later the analysis was extended by considering d-wave pairing which indeed turns out to be favored when the local repulsion is sizable.¹⁷ Our following analysis of the symmetry of the order parameter in a two-dimensional system near a PS shares many features with the analysis of Ref. 17, even though the model considered in Ref. 17 assumes that the small-q attraction is of pure phononic origin with no connection with PS.¹⁸

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In the proximity of PS the effective interaction has a rich dynamical structure which is relevant for the anomalous behavior above T_c .⁵ Concerning the superconducting properties we limit ourselves to consider the static part of this effective interaction which has the form⁵

$$V_{\rm eff}^{\rm PS}(q_x, q_y) = U - \frac{V}{\kappa^2 + q_x^2 + q_y^2},$$
 (1)

where κ is the cutoff of the attractive interaction, *V* is the attraction strength in unity of the inverse square of the lattice constant, and *U* is an on-site effective repulsion;¹⁹ we impose on the interaction the periodicity of the lattice without modifing the behavior at small *q* by writing $q_x^2 + q_y^2$ as $2[2 - (\cos(q_x) + \cos(q_y))]$. Near PS κ^2 vanishes as $\delta \rightarrow \delta_c^{\text{PS}}$ where δ is the doping (with respect to half filling) and δ_c^{PS} is the critical doping at which the instability for PS occurs. At δ_c^{PS} the value *V* stays finite and a singular effective attraction at small *q* arises.

To study the symmetry of the superconducting gap we solve a simple BCS self-consistent equation for the gap parameter $\Delta(\vec{k})$,

$$\Delta(\vec{k}) = -\frac{1}{N} \sum_{\vec{p}} V_{\text{eff}}(\vec{k} - \vec{p}) \frac{\tanh(\epsilon_{\vec{p}}/2T)}{2\epsilon_{\vec{p}}} \Delta(\vec{p}), \qquad (2)$$

with $V_{\text{eff}} = V_{\text{eff}}^{\text{PS}}$ given in Eq. (1). Later we shall use a different effective potential $[=V_{\text{eff}}^{\text{CDW}}$; see following Eq. (7)] to analyze the gap in the proximity of a CDW.

Of course, approaching δ_c^{PS} the superconducting properties obtained within the BCS theory should only be considered on a qualitative ground. For instance, wave function corrections become relevant. (The same comment would apply for $\delta \rightarrow \delta_c^{\text{CDW}}$, where δ_c^{CDW} is the critical doping for the CDW instability.) However, it is worth noting that vertex corrections could partially compensate wave function corrections due to small-q scattering similarly to what happens in one dimension,^{20,21} or near one dimension.²² An explicit calculation has indeed shown that the superconducting critical temperature is enhanced by considering the vertex corrections to Migdal-Eliashberg theory in a model with small-q coupling to optical phonons.²³

In Eq. (2) the sum over \vec{p} is done over the first Brillouin zone, N is the number of lattice sites, and $\epsilon_{\vec{k}}^2 = \xi_{\vec{k}}^2 + \Delta_{\vec{k}}^2$ with $\xi_{\vec{k}}$ being the electronic dispersion measured with respect to the Fermi energy E_F . We consider a tight-binding model with hopping up to the fifth nearest neighbors,

$$\xi(k_x, k_y) = \sum_{i=1}^{6} c_i \eta_i(k_x, k_y),$$
(3)

where, according to Ref. 24, we choose $\eta_1(k_x,k_y)=1$, $c_1=0.1305$ eV, $\eta_2(k_x,k_y)=\frac{1}{2}[\cos(k_x)+\cos(k_y)]$, $c_2=-0.5951$ eV, $\eta_3(k_x,k_y)=\cos k_x \cos k_y$, $c_3=0.1636$ eV, $\eta_4(k_x,k_y)=\frac{1}{2}(\cos 2k_x+\cos 2k_y)$, $c_4=-0.0519$ eV, $\eta_5(k_x,k_y)=\frac{1}{2}(\cos 2k_x\cos k_y+\cos 2k_y\cos k_x)$, $c_5=-0.1117$ eV, $\eta_6(k_x,k_y)=\cos 2k_x\cos 2k_y$, and $c_6=0.0510$ eV. These parameters are appropriate for the band structure of the Bi-2212 compounds, thus giving an open Fermi surface and a van Hove singularity (VHS) slightly below the Fermi level (for electrons). The value of $E_F = -c_1 = -0.1305$ eV is fixed to get the proper distance of the Fermi surface from the VHS ($E_F - E_{VHS} = 35$ meV as determined experimentally), and corresponds to (optimal) doping $\delta = 0.17$. The full bandwidth W is 1.4 eV.

The choice of the parameters entering the effective interaction $V_{\text{eff}}^{\text{PS}}$ is to some extent arbitrary since they will depend on the specific mechanism driving PS. We choose V=0.21W=0.3 eV and U=0.2 eV. These values are of the order of magnitude of the estimates obtained for a singleband Hubbard-Holstein model near PS.^{13,5}

The BCS equation (2) is solved in two limiting cases: (i) at zero temperature, to obtain the ground state in the superconducting phase, and (ii) in the linearized form, for $\Delta(\vec{k})$ going to zero, to evaluate the critical temperature T_c of the superconducting transition. We provide a numerical selfconsistent solution of the BCS equation on a lattice of $N=128\times128$ points (in each quadrant of the Brillouin zone), taking advantage of the fast Fourier transform.^{25,26} In the case of an undistorted tetragonal lattice, both in the proximity to PS and to CDW, the solutions in the *s*-wave and *d*-wave channels are decoupled and the solution is a superposition of all harmonics of a given symmetry. In the range of parameters we have considered the *s*-wave solutions can be roughly approximated by a linear combination of the first square harmonics,

$$\Delta_s(\vec{k}) \simeq \Delta_0 + \Delta_1(\cos k_x + \cos k_y) + \Delta_2 \cos k_x \cos k_y + \cdots,$$
(4)

while the *d*-wave solutions are decoupled in the $d_{x^2-y^2}$ -like and d_{xy} -like harmonics

$$\Delta_{d_{x^2-y^2}}(\vec{k}) \simeq \Delta_1(\cos k_x - \cos k_y) + \cdots, \qquad (5)$$

$$\Delta_{d_{yy}}(\vec{k}) \simeq \Delta_1 \sin k_x \sin k_y + \cdots.$$
 (6)

In all cases we find that the d_{xy} -like solution is strongly suppressed because it has a line of nodes along the relevant $\Gamma \overline{M}$ directions where saddle points are present at $(\pm \pi, 0)$, $(0, \pm \pi)$, giving rise to van Hove singularities in the density of states.²⁷

We now proceed to analyze the gap parameter at T=0 K in the proximity of PS. The solution is given for the same set of parameters at varius κ 's. In Fig. 1(a) we show the momentum dependence of the s-wave solution on the Fermi surface. We define an angular variable ϕ measured from the line MY to detect the points on the Fermi surface as seen from the point $Y \equiv (\pi, \pi)$. The s-wave solution has two nodes in each quadrant, symmetrically located with respect to the ΓY direction (as in Ref. 14), whose positions depend on κ . The maximum value of the gap is in the ΓM directions, near the van Hove singularities (this is due to almost complete momentum decoupling at small q). In Fig. 1(b) we show the same ϕ dependence for the $d_{x^2-y^2}$ solution. This solution has a line of nodes along the ΓY direction $(\phi = 45^{\circ})$ and the maximum value along ΓM directions. The maximum value of the gap parameter is much larger for the *d*-wave solution than for the *s*-wave solution and the relative



FIG. 1. Angular dependence of the order parameter normalized by its maximum value for various cutoffs κ of the attractive interaction close to PS [Eq. (1)]. U=0.2 eV and V=0.3 eV. The angle ϕ is defined in the inset, where the Fermi surface branch in the upper right quadrant of the Brillouin zone is shown. (a) Angular dependence of the *s*-wave order parameter normalized by its maximum value $\Delta_{\max}^s = 237.9$, 161.1, and 9.4 K for $\kappa = \pi/20$, $\pi/16$, $\pi/8$, respectively; (b) angular dependence of the *d* wave normalized order parameter with $\Delta_{\max}^d = 358.6$, 308.0, and 85.8 K for $\kappa = \pi/20$, $\pi/16$, and $\pi/8$, respectively. The pure *d*-wave solution (dot-dashed line) and a weaker coupling (V=0.1 eV) (long-dashed line to be discussed later) solution are also shown.

difference is so neat that it is easy to predict also a large difference in the condensation energy.

The comparison between the *s*-wave and *d*-wave solutions is completed evaluating the condensation energy per particle $\delta F \equiv F_{super} - F_{normal}$ for the BCS ground state. In Fig. 2 we report the results for the two analyzed symmetries and different κ 's. The difference between the two condensation energies is considerable, since we find $\delta F_d / \delta F_s > 3.5$ for all considered κ 's.

From the above analysis it is clear that the *d*-wave solution is the favorite gap parameter of the superconducting phase induced by the interaction (1) characteristic of models that present a small-momentum charge instability. We would like to point out that this result is a consequence of three related but distinct features of the system: First there is a strongly *q*-dependent attraction peaked at small momenta. This leads to a momentum decoupling so that the *modulus* of the gap parameter tends to match the local density of states of the system. Then a second feature needed to obtain a gap



FIG. 2. *s*-wave (solid line) and *d*-wave (dashed line) condensation energy per particle $\delta F \equiv F_{\text{super}} - F_{\text{normal}}$ as a function of κ . U = 0.2 eV and V = 0.3 eV.

anisotropy is a largely anisotropic density of states, possibly with extended van Hove singularities in some regions of the k space. Both these features, however, only point towards the setting in of an anisotropic order parameter, which still could well be of the s type. It is the presence of a (nearly) momentum-independent sizable repulsion which leads to dwave symmetry. This solution is able to avoid the isotropic repulsive interaction U since its average over the Brillouin zone is zero while keeping the paired electrons in the attractive region of the effective potential. Roughly, the *d*-wave becomes favorable when the average repulsion felt by the s-wave paired electrons exceeds the loss in condensation energy due to the vanishing of the order parameter along the nodal regions. Among the d waves, the $d_{x^2-y^2}$ is preferred because the nodes occur where the modulus of the order parameter is anyway small (i.e., due to momentum decoupling, where the density of states is small). As extensively discussed in the Appendix, by reducing the relative value of U with respect to V the s-wave solution may be recovered. At $\kappa = \pi/16$ we find that this happens for $U^* = 0.06$ eV. We believe, however, that the presence of a sizable $U > U^*$ is an unavoidable feature of strongly correlated systems. In turn strong correlation is a prerequisite for the likely occurrence of a charge instability and for the related enhancement of the residual attraction among quasiparticles. This leads to the conclusion that pairing near PS in strongly correlated systems is of $d_{x^2-y^2}$ -wave symmetry.

Notice that in the presence of an attraction like the one given in Eq. (1) many other channels (besides $d_{x^2-y^2}$ and s) are unstable with respect to pairing. In particular triplet p and singlet d_{xy} waves should also be considered. However, by evaluating their (free) energy we obtain that $d_{x^2-y^2}$ is always preferred. We also find that, whereas the d_{yy} -wave solution is generically quite high in energy, p-wave solutions have an energy comparable with or lower than s-wave solutions only for U > 0.2 eV, while they have higher energy for U < 0.2 eV. To be more specific, for a typical parameter set $(\kappa = \pi/16, V = 0.3 \text{ eV} \text{ and } U = 0.2 \text{ eV})$, we find that the condensation energy $\delta F = -0.191, -0.627, -0.752$ eV for the d_{xy} , p_x , and $p_x - p_y$ solutions, respectively. These condensation energies should be compared with the analogous quantities in the case of $d_{x^2-y^2}$ and s waves, which are $\delta F_{d_{x^2-y^2}} = -3.276 \text{ eV}$ and $\delta F_s = -0.618 \text{ eV}$.

III. PROXIMITY TO CDW'S

The occurrence of PS is a theoretical outcome of models with short-range forces. In a real charged system long-range forces prevent charge segregation on a macroscopic scale, leaving open the way to charge segregation on a microscopic scale, i.e., to CDW's.²⁸ If and when CDW's are realized is a debated issue. In the early stage of the investigation into this problem, a charge-glass behavior was suggested as a result of frustated PS.²⁹ Recently, CDW's have been observed in the related compound La1,48Nd0,4Sr0,12CuO4.30 Superstructures31 and in-plane CDW's have also been observed in various cuprates.³² It is not yet clear whether this experimental evidence can indeed be attributed to the interplay between PS and long-range Coulomb forces. Here we assume that the system is near a CDW instability characterized by an incommensurate wave vector $q_{\rm CDW}$. The value of this $q_{\rm CDW}$ is mainly fixed by the balance between charge segregation favored by short-range forces and the consequent electrostatic cost. To a large extent, q_{CDW} is not a Fermi surface property (i.e., q_{CDW} is not a nesting vector). In the analysis of the Hubbard-Holstein model q_{CDW} is found almost parallel to the $(\pm \pi, 0), (0, \pm \pi)$ directions (similarly to the finding of Ref. 33 in the analysis of an effective Ising model with longrange forces). Its value comes out to be of order 1.

Near the CDW instability and neglecting the dynamics relevant to the anomalous properties above T_c , the effective interaction among quasiparticles can be written as⁵

$$V_{\rm eff}^{\rm CDW}(q_x, q_y) = U - \frac{1}{4} \sum \frac{V}{\kappa^2 + \omega_q^{\alpha}}, \qquad (7)$$

where the sum is over the four equivalent vectors of the CDW instability $q^{\alpha} = (\pm q_{\text{CDW}}, 0), (0, \pm q_{\text{CDW}})$ and $\omega_q^{\alpha} = 2[2 - \cos(q_x - q_x^{\alpha}) - \cos(q_y - q_y^{\alpha})]$. This expression is used to reproduce the behavior $\sim -1/[\kappa^2 + (q_x - q_x^{\alpha})^2 + (q_y - q_y^{\alpha})^2]$ for $q \rightarrow q^{\alpha}$ while mantaining the lattice periodicity.

As in Eq. (1), κ acts as a cutoff of the effective interaction. It can be identified with the inverse correlation length of the CDW and vanishes at δ_c^{CDW} . We take for *U* and *V* the same values used before³⁴ and solve Eq. (2) with $V_{\text{eff}} = V_{\text{eff}}^{\text{CDW}}$ given in Eq. (7).

All the qualitative features presented above for the case of proximity to PS are not changed near the CDW instability if q_{CDW} is small, specifically if it stays smaller than the momentum q_F^* connecting the two branches of the Fermi surface around the VHS. For the considered set of band parameters we find $q_F^*=1.2$. We report in Fig. 3, the values of the gap on the Fermi surface as a function of the angle ϕ for $q_{\text{CDW}}=0.9$ both for *s*- and *d*-wave symmetry. Notice that for all $q_{\text{CDW}} < q_F^*$ the shape of the *d*-wave gap is not very different from a pure $d_{x^2-y^2}$ [dot-dashed line in Fig. 3(b)]. The situation would be different if we would consider a much smaller value for the attraction *V* (say, $V \approx 0.2 \text{ eV}$), pushing the system in a weak-coupling regime. In this case there is a tendency of the curve to become flat around $\phi = \pi/4$ analo-



FIG. 3. Angular dependence of the order parameter normalized by its maximum value for various cutoffs κ of the attractive interaction close to a CDW instability [Eq. (7)]. U=0.2 eV and V=0.3 eV. (a) *s*-wave order parameter normalized by its maximum value $\Delta_{\max}^s = 17.5$, 5.9, and 1.3 K for $\kappa = \pi/20$, $\pi/16$, and $\pi/12$, respectively; (b) *d*-wave normalized order parameter. with $\Delta_{\max}^d = 200.0$, 136.4, 21.5 K for $\kappa = \pi/20$, $\pi/16$, and $\pi/8$, respectively. The pure *d*-wave solution (dot-dashed line) and a weaker couplig (V=0.2 eV and $\kappa = \pi/16$) (long-dashed line) solution are also shown.

gously to the finding of Ref. 17 [dotted curve in Fig. 3(b) and, even more evidently, for V=0.1 eV in Fig. 1(b)].

For $q_{\text{CDW}} > q_F^*$ a new feature appears in Δ_k . As shown in Fig. 4, where we report the gap for various values of $q_{\rm CDW}$, by increasing $q_{\rm CDW}$ extended flat regions develop around the maxima at $\phi = 0, \pi/2$, which eventually become local minima for the *d*-wave solution. This feature is very pronounced for small κ ($\kappa = \pi/16$ in Fig. 4). The reason is the interplay between the VHS, which mostly weigh $\phi = 0, \pi/2$, and the value of q_{CDW} which for $q_{CDW} > q_F^*$ only connects the two branches of the Fermi surface around the VHS at finite values of ϕ , resulting in maxima for Δ_{k} near these values of ϕ . Notice that these local maxima in the order parameter are much more pronounced in the s-wave [Fig. 4(a)] than in the *d*-wave channel (Fig. 4b). Moreover, in the s-wave order parameter they are also visible when $q_{\rm CDW} < q_F^*$ provided the mass term κ^2 is large enough $(\kappa > \pi/12)$. In this latter case, although the instability wave vector is not large enough to encompass two branches of the Fermi surface, the attractive potential is broad and shallow



FIG. 4. (a) Angular dependence of the *s*-wave normalized order parameter in the proximity of a CDW instabilities with different values of q_{CDW} . U=0.2 eV, V=0.3 eV, and $\kappa^2 = \pi/16$; (b) same as (a) for *d*-wave symmetry.

enough to "put in touch" substantial momentum regions on the different branches to build up an increased order parameter at finite values of ϕ away from $\phi = 0, \pi/2$.

Finally we considered an *isotropic* CDW instability.³⁵ In this latter case the effective attraction is approximately given by

$$-\frac{(V/4)}{\kappa^2 + |\mathbf{q} - \mathbf{q}_{\text{CDW}}|^2}.$$
(8)

Then we write $|\mathbf{q} - \mathbf{q}_{\text{CDW}}|^2 \approx \{2[2 - \cos(q_x) - \cos(q_y)]^{1/2} - q_{\text{CDW}}\}^2$ to guarantee the correct lattice periodicity, while keeping the presence of a line of q points with a large attraction. The result is given in Fig. 5 for the case of d-wave symmetry only and for various values of q_{CDW} . It is apparent that the feature of the local minima at $\phi = 0, \pi/2$ is *less* pronounced since more q's are effective in connecting different points on the Fermi surface.

To our knowledge there is no report in the literature of local minima for the gap at $\phi = 0, \pi/2$. This would imply that the q_{CDW} invoked to describe cuprates has to be smaller than q_F^* , or the instability should have an almost isotropic structure. It is worth noting that in the Hubbard-Holstein model⁵ the effective attraction is indeed diverging in an anisotropic way at $\delta = \delta_c^{\text{CDW}}$; however, it has a large value all over the



FIG. 5. Same as in Fig. 4(b), but using the potential for an *isotropic* CDW [Eq. (8)].

region $q \approx q_{\text{CDW}}$. In this case we get an intermediate behavior between the anisotropic and isotropic CDW's.

In the above discussion of the behavior of the gap near CDW's we have only partially commented on the *s*-wave solution which also presents rich structures depending on q_{CDW} [Figs. 3(a) and 4(a)]. Indeed we find that the stable solution at T=0 is *d* wave even in the proximity to CDW's similarly to the PS case, provided a sizable U ($\approx 0.2 \text{ eV}$, according to our choice) is present. This can be inferred from the larger values of the maximum of the *d*-wave gap with respect to the *s*-wave gap. The explicit computation of the condensation energy confirms this expectation in all the considered cases. As an example, in Fig. 6, we report δF for the set of parameters corresponding to Fig. 4.

For completeness we have also carried out in the Appendix systematic analysis of the relative stability of *s*- versus *d*-wave solutions in order to find the influence of the various parameters (mainly κ^2 and q_{CDW}) in determining the symmetry of the gap function.

IV. T_c vs DOPING

The evaluation of a reliable superconducting critical temperature is the most difficult issue of a theory dealing with singular interactions like those generated nearby PS and CDW's. In the present analysis we start by solving Eq. (2) in the linearized form in order to get T_c vs κ^2 in the proximity of PS or CDW's (depending on $V_{\text{eff}} = V_{\text{eff}}^{\text{PS}}$ or $V_{\text{eff}} = V_{\text{eff}}^{\text{CDW}}$).

We report in Fig. 7 the evaluated critical temperature for the set of parameters discussed above and for different κ smaller than the Fermi wave vector k_F . We have verified that the *d*-wave transition has always a substantially larger critical temperature than the *s*-wave transition (not reported in Fig. 7) both in the proximity of PS and CDW's. Roughly, the maximum value of the BCS gap (at T=0) gives the order of magnitude of the correponding $T_c (\simeq \Delta_{max}/2)$. The curves show a strong dependence on κ^2 , which at small κ^2 assumes the form $T_c \simeq -\ln \kappa^2$.

The above evaluations of T_c lead to the unphysical result that $T_c \rightarrow \infty$ for $\delta \rightarrow \delta_c^{\text{PS}}$, δ_c^{CDW} , since in these limits κ^2 vanishes and the effective potential diverges with a nonintegrable power. The inclusion of the dynamical effects beyond BCS would cut off the divergency of T_c . However, even



FIG. 6. *s*-wave (solid line) and *d*-wave (dashed line) condensation energy per particle $\delta F \equiv F_{\text{super}} - F_{\text{normal}}$ as a function of the modulus of the CDW wave vector. U=0.2 eV, V=0.3 eV, and $\kappa^2 = \pi/16$.

within the present BCS approach, the singularity is cut off by considering that κ^2 , being the square of an inverse correlation length, is vanishing at δ_c only at T=0. From the theory of quantum critical points (QCP's),^{36–38} it follows that κ^2 becomes a finite function of T for $T>const\times(\delta-\delta_c)^{\beta z/(d+z-2)}$, where d is the dimension, z is the dynamical critical index, and β is the index of the "mass" κ^2 at T=0, $\kappa^2 \sim (\delta-\delta_c)^{\beta}$. This indicates that when PS or CDW's occur at finite temperature, they will occur at $\delta_c(T) < \delta_c(0) \equiv \delta_c$. Roughly we can write

$$\kappa^2 = \max(a(\delta - \delta_c)^{\beta}, bT^{(d+z-2)/z}), \qquad (9)$$

with *a* and *b* model-dependent positive constants, in order to represent the (much more complex) crossover of the actual $\kappa^2(\delta - \delta_c, T)$. Here we will not consider the influence of superconductivity on the underlying normal phase transition (PS or CDW's). This effect would provide an additional "mass" contribution expressing the stabilizing effect of superconductivity on PS and CDW's.³⁹ The proper *z*'s are *z*=3 for PS and *z*=2 for CDW's as one can see from the inspection of the fluctuation propagator⁵. In *d*=2 their values are indeed immaterial since in both cases the above equation reduces to $\kappa^2 = \max(a(\delta - \delta_c)^\beta, bT)$. Dimension 2 is also peculiar because of logarithmic corrections leading to $\kappa^2 \simeq a' T[1 + O(\ln T, \ln(\delta - \delta_c)]$. This holds in the so-called classical gaussian region³⁸ $T > (a/b)(\delta - \delta_c)^\beta$.

Concerning the index β , for a QCP one would expect $\beta = 2\nu = 1$, $\nu = 1/2$ being the classical Gaussian index of the inverse correlation length.⁴⁰

However, PS is a first-order transition since symmetry does allow the presence of cubic terms (the order parameter being a scalar, density deviation, at q=0). In the parameter space (doping δ versus bare interaction coupling g, for instance, the electron-phonon coupling in the Hubbard-Holstein model⁵ or the nearest-neighbor interaction V in the excitonic model^{8,41}) the Maxwell construction will lead to first-order transitions between stable phases with $\kappa^2 > 0$. Depending on the models considered, the first-order transition could end at a critical point where PS is second order. Around this point, which has a fixed value for both δ and



FIG. 7. *d*-wave critical temperatures as a function of the the mass parameter κ^2 close to the PS instability for V=0.3 eV (solid line) and to the (anisotropic) CDW instability with $q_{CDW}=0.9$ and V=0.3 eV (dashed line) and V=0.45 eV (dot-dashed line).

g, one would get $\kappa^2 \sim (\delta - \delta_c)^2$, i.e., $\beta = 2$. If the transition is weakly first order (i.e., $\kappa^2 \ll 1$), one could also analyze the case $\beta = 1$ for PS.

The incommensurate CDW is usually of second order since cubic terms are not allowed by momentum conservation. There can be exceptions when q_{CDW} is extremely small or when $q_{\text{CDW}} \approx 2k_F$.⁴² For the CDW considered in our analysis we assume a second-order transition and we take $\beta = 1$.

From the dependence of $\kappa^2 \equiv \kappa^2(\delta - \delta_c, T)$ and Fig. 7 for $T_c(\kappa^2)$ we see that $T_c(\simeq T_c[\kappa^2(\delta - \delta_c, T=0)])$ will rapidly increase by decreasing doping towards δ_c until the value $T_c^* \sim (a/b)^{z/(d+z-2)}(\delta - \delta_c)^{\beta z/(d+z-2)}$ $[T_c^* = (a/b)(\delta - \delta_c)^\beta$ in d=2] is reached at a doping δ^* . Then T_c will slowly approach the value (still of order $\sim T_c^*$) which solves the equation

$$T_c = T_c [\kappa^2 (\delta - \delta_c = 0, T_c)].$$

In the case $\beta = 1$ and d = 2, this plateau will cover all the classical Gaussian region $\delta_{GL}(T_c) < \delta < \delta^*$ (GL stands for Ginzburg-Landau). Here $\delta_{GL}(T) < \delta_c(T=0)$ is the boundary of the region where critical fluctuations start to be relevant³⁸ before arriving at the actual critical doping $\delta_c(T)$ for the normal phase transitions (PS or CDW's), if any. The classical Gaussian region $\delta_{GL}(T_c) < \delta < \delta^*$ could be very small and indeed this is the case if the coefficient *a* is large. In the Hubbard-Holstein model we estimate $a \approx 10-30$. On the other hand, assuming from Fig. 7 that at optimal doping $\kappa_{opt}^2 = 0.1$ and $\kappa_{opt}^2 \approx a(\delta^* - \delta_c) \approx bT_c^{max}$, we would get $(\delta^* - \delta_{GL}) \approx (\delta^* - \delta_c) \approx \kappa_{opt}^2/a \approx 0.01$. However, because of the two-dimensional nature of our system, there will be a larger region of doping $\delta < \delta_{GL}$ before arriving at the normal phase transition. This region will be governed by quantum fluctuations around the ordered state at $T=0.^{38}$

We suggest that T_c will be a slowly varying function of doping in this region, since κ^2 will mainly depend on temperature. Eventually T_c will drop when the normal phase transition takes place or the effects of proximity to the charge instability are no longer effective. In the case $\beta=2$ it can also happen that the T=0 critical point is isolated; i.e., no PS



FIG. 8. Doping dependence of the superconducting critical temperature T_c for a fixed value of the mass parameter $\kappa^2 = 0.1$. The dotted line is for the case of proximity to PS (with V=0.32 eV) and the dashed line is for proximity to a CDW instability with $|\mathbf{q}_{\text{CDW}}|=0.9$ and V=0.45 eV. In both cases the VHS is at $\delta=0.355$ and U=0.2 eV. The solid line is an estimate of T_c by assuming a doping dependence of κ^2 according to Eq. (9) for d=2 and $\beta=1$ in the CDW case.

instability exists, but for $\delta = \delta_c$ and T = 0. Then we expect a symmetrical behavior at $\delta < \delta_c$ with respect to $\delta > \delta_c$, and the superconducting T_c will fastly decrease as soon as $(\delta - \delta_c)^2 > (\delta^* - \delta_c)^2$ with $\delta < \delta_c$.

Notice that in discussing T_c versus doping we have assumed that the main doping dependence is via κ^2 . Indeed we have verified that the variations induced by moving E_F are less relevant. In Fig. 8 we report the variation of T_c by varying doping at fixed κ^2 and by assuming a doping dependence of κ^2 according to Eq. (9). Specifically, $\kappa_{opt}^2 \approx 0.1$ and $\kappa^2 = bT$ for $\delta < \delta_c$. Analogous results are obtained for $\Delta_{\rm max}$ versus doping. At fixed κ^2 , the greatest values for T_c are obtained for $E_F \simeq E_{\text{VHS}}$. Then, a vanishing Δ_{max} and T_c are obtained for very high doping ($\delta > 0.6$) or very small (or even negative) doping. This analysis is only indicative, since the rigid band picture is not valid approaching half-filling, where a metal-insulator transition takes place and antiferromagnetism appears. Nevertheless, it correctly describes the rather natural argument that the VHS tends to pin the Fermi level,⁴³ which then requires large changes in the filling to be sensibly affected. Then all properties which do not directly depend on the rapidly varying shape of the Fermi surface (like, e.g., nesting) are rather slowly varying functions of the doping. These arguments therefore suggest that strong variations of T_c with doping, like those observed in many cuprates, are hardly obtained in terms of a dependence on band parameters (specifically, tuning the VHS), while they are quite natural in the context of proximity to an instability, where doping will control the effective potential itself and not only the density of states. This strong variation is indeed found when T_c is evaluated by allowing κ^2 to be doping dependent (solid line in Fig. 8 to be contrasted to the smooth variation of the dotted and dashed curves). Notice that our optimal doping value is fixed by proximity to the charge instability and not by the proximity to the VHS. This generically agrees with the experimental finding that at the maximum T_c the VHS is not at the Fermi energy but below it.⁴⁴

V. CONCLUSION

In this paper we have analyzed the symmetry of the superconducting order parameter in the proximity of PS and CDW instabilities. We have found that *d*-wave pairing is favored in both cases provided a q-independent repulsion $U>U^*$ is present in the effective interaction among quasiparticles. In the CDW case the instability wave vector $q_{\rm CDW}$ should be substantially smaller than the wave vectors of the reciprocal lattice. An s-wave solution is realized for $U \le U^*$ depending on q_{CDW} and location of the VHS. However, when the s-wave solution is stable, it does not present nodes on the Fermi surface both in the proximity of PS and CDW's in agreement with the finding of Ref. 17. We have considered the band parameters appropriate for BiSCCO; however, we have found analogous results (not reported in the paper) by using the parameters of YBCO as given in Ref. 6.

Notice that our static analysis could somewhat overestimate the effects of the repulsive U. However, for the range of parameters considered in Secs. II and III, the maximal values U^* compatible with a (anisotropic) *s*-wave superconductivity ground state solution are so small (always smaller than 0.1 eV) that it is implausible that dynamical screening would reduce U below these values, thus changing our conclusions on the stability of *d*-wave pairing with respect to *s*-wave pairing.

Disorder is an other relevant mechanism which affects the relative stability of the d- and s-wave superconducting phases: s-wave superconducting is more robust in this respect and large disorder could favor this latter symmetry with respect to the d-wave phase. This issue was recently considered in Ref. 45 and was not of our concern in the present paper.

Concerning the superconducting critical temperature T_c , we have seen that the most important parameter controlling its value is κ^2 , even though the VHS produces a sizable enhancement, which, however, would be effective in a too extended region of doping. The doping dependence of κ^2 reduces this region and leads to a strong dependence of T_c on doping. The maximum T_c is not directly related to the proximity to a VHS, but it is located just above the QCP for the charge instability. Assuming a CDW instability, within the range of parameters we have considered (allowing for larger values of V within a factor of 2), $\kappa^2 \approx 0.1-0.2$ is enough to get $T_c \approx 100$ K. These values of κ^2 correspond to correlation lengths of the order of 2–3 lattice constants.

The PS and CDW scenarios have various analogies with the antiferromagnetic spin fluctuation (AF) scenario.^{6,37,46} Indeed both approaches assume the proximity to a QCP. A main claim is that the AF scenario is supported by a large amount of experimental evidence, first of all the actual existence of a AF transition. However, notice that the experimental T_c^{max} is obtained at a doping far away from δ_c^{AF} . Moreover, according to Ref. 47, two remarkable crossover lines can be identified in the phase diagram of the superconducting cuprates. The first one identifies the doping dependence of the maximum in the uniform magnetic susceptibility (T_{cr}). The second one ($T_* < T_{\text{cr}}$) separates the quantum critical from the quantum disordered regimes.⁴⁸ These two curves do not cross, but rather converge towards the same point (Figs. 2 and 3 in Ref. 47) nearby the optimal doping. It



FIG. 9. Schematic phase diagram for the high-temperature superconducting cuprates. Both the AF and CDW quantum critical points (solid dots) are shown on the zero-temperature axis. The T_* line of Ref. 47 is also indicated by the dashed line. The antiferromagnetic (AF), superconducting (SC) phases, and the spin quantum-disordered (SQD) regime are also indicated. The crossover line is shaded and phase-transition lines are solid.

is quite tempting to relate this remarkable point with the zero-temperature CDW quantum critical point. Indeed, according to our analysis, this point should be close to the optimally doped regime.

Within this scheme, the existence of PS or CDW's (once long-range forces are taken into account) is not an alternative to the existence of an AF QCP and the two QCP's control the behavior of the system at different dopings. The CDW sets up the maximum critical temperature and can constitute the substrate to substain AF fluctuations far away from the ordered phase, by allowing for hole-rich and hole-poor "stripes." A constructive interplay between CDW's and AF's was also suggested in Ref. 29 within the analysis of the *t-J* model. The criticism that the experimental J ($\simeq 0.12$ eV $\simeq 0.2t$) is lower than the value needed for PS ($J \simeq t$) (Ref. 49) can be overcome by considering additional sources for charge instabilities (for instance, coupling to the lattice^{5,12,13} or charge-transfer excitons⁸⁻¹⁰). With the assumption that the maximal T_c is associated with the CDW quantum critical point, independently of the underlying instability mechanism, the quantum-disordered phase will correspond to the region between the AF and CDW quantum critical points. Figure 9 represents this scenario in a schematic way.

According to the above scenario, the occurrence in the phase diagram of the high-temperature superconducting cuprates of both an AF (at low doping) and a CDW (at intermediate doping) quantum critical point and the related existance of two correlation lengths ξ^{AF} and ξ^{CDW} opens new possibilities for the interpretation of various effects related to the magnetic correlations like, e.g., the presence of a spin gap at low and intermediate doping, the behavior of the spin-spin correlation length, and the discrepancies existing between NMR and neutron scattering experiments.⁵⁰ In particular, in the spin quantum-disordered regime it is natural to infer the existence of a spin gap as a property of spin waves in inhomogeneous systems, as also reported in Ref. 29.

Within the proposed scenario, owing to the crucial role played by CDW fluctuations in determining the physics of the superconducting cuprates, it is quite relevant whether an incommensurate CDW symmetry breaking occurs. In this context, the quasi-two-dimensional character of the cuprates could play a role in (partially or totally) suppressing the critical temperature for the establishing of a static incommensurate long-range CDW order for which a two-component order parameter is required. If the low dimensionality prevents the establishing in the cuprates of incommensurate long-range CDW order on a macroscopic scale, one is left with the possibility of order on a mesoscopic scale or slow dynamical fluctuations.⁵¹ This locally (in space and/or time) "ordered" phase should then be identified with the magnetic quantum-disordered region below T_* .

A true CDW order can occur when a suitable matching between the underlying lattice and the charge fluctuations produces commensurability conditions and a consequent pinning. It was recently proposed³⁰ that such an occurrence takes place in $La_{2-x-y}Nd_ySr_xCuO_4$ at 1/8 doping. Remarkably, in this systems, the pinned charge order and the consequent insulating behavior take place before a long-range AF order is established.³⁰ This is a clear indication that the freezing of charge fluctuations is responsible for the insulating behavior rather than the magnetic ordering. Of course this does not rule out the possibility of magnetic interactions being (co-)responsible for the charge instability, the origin of which (magnetic, excitonic, phononic, or a combination of these mechanisms) is still an open issue.

The scenario proposed in this paper relates (d-wave) superconductivity and anomalous normal state behavior⁵ to the proximity to a charge instability. This mechanism is quite general and is likely expected to work in other systems than the high-temperature superconducting cuprates. A superconducting phase close to both incommensurate SDW (Ref. 52) and CDW (Ref. 53) phases occur in some nearly one-dimensional systems, thus suggesting also in this case a relation between superconductivity and an incommensurate instability.

Finally we would like to mention that superconductivity at a fairly large critical temperature ($T_c = 31$ K) occurs in $Ba_{1-r}K_rBiO_3$ systems close to a CDW phase. This phase at low potassium doping is commensurate and responsible for the insulating behavior of the system. However, by increasing the doping the system becomes metallic and superconducting. Interestingly enough, optical experiments⁵⁴ show that the feature in the optical conductivity related to the CDW gap in the insulating phase smoothly and continuously shifts at lower frequencies upon doping and persists in the midinfrared region in the metallic phase, where it coexists with the Drude contribution. It is obviously quite tempting to interpret these results as an indication of persistance of CDW incommensurate fluctuations in the metallic phase. If this were the case, the scenario proposed here could be of relevance for these systems as well.

APPENDIX

As mentioned in Secs. II and III, a crucial role in the relative stability of the *d*-wave vs anisotropic *s*-wave superconducting phases is played by the local residual repulsion between the quasiparticles *U*. In particular, for a given parameter set (V, κ , q_{CDW}) it is possible to find a critical U^* above which *s*-wave superconductivity becomes unstable with respect to the *d*-wave phase. This quantity is therefore

TABLE I. Dependence of the normalized critical U^* on the mass parameter κ close to a PS and on the modulus of the instability wave vector close to the CDW instability (for $\kappa^2 = \pi/16$). PS CDW(1,0) CDW(1,1) CDW_{iso}

PS		CDW(1,0)		CDW(1,1)		CDW _{iso}	
к π/16	$U^*/\langle V \rangle$ 0.35	q _{CDW} 0.9	$U^*/\langle V \rangle$ 0.40	q _{CDW} 0.9	$U^*\langle V \rangle$ 0.42	q _{CDW} 0.9	$U^*\langle V \rangle$ 0.29
$\pi/8$	0.42	1.2	0.45	1.2	0.49	1.2	0.42
$\pi/4$	0.51	1.5 1.8	0.52 0.56	1.5 1.8	0.59 0.74	1.5	0.59

directly related to and provides information on the relative robustness of the two superconducting phases: the larger U^* is and the more difficult it is to spoil *s*-wave superconductivity. In order to filter this information from the absolute strength of superconductivity for a given parameter set, we normalize the U^* with $\langle V_{\text{attr}}(q_x, q_y) \rangle$, the average value (on the Brillouin zone) of the attractive part of the effective potentials in Eqs. (1) and (7).

We carried out an analysis of the normalized critical local repulsion $U^*/\langle V_{\text{attr}}(q_x, q_y) \rangle$ as a function of the mass parameter κ^2 for the PS instability, and as a function of the wavelength for the CDW instabilities with wave vectors in the (1,0) and (1,1) directions and for the isotropic CDW. Table I displays the results of this analysis. Two clear tendencies are found. First of all the *s*-wave solution is made more stable $[U^*/\langle V_{\text{attr}}(q_x, q_y) \rangle$ increases] by increasing the κ^2 . This is because in this way the effective potential becomes less sharply structured in momentum space, the attractive well being more shallow. As a consequence, the superconducting gap anisotropy is less pronounced (there is a

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weaker momentum decoupling), making it in turn comparatively less favorable to create a line of nodes in the order parameter to produce *d*-wave superconductivity.

The second clear tendency is the increase of $U^*/\langle V_{\text{attr}}(q_x, q_y) \rangle$ by increasing the momentum of the CDW instability. Increasing $|q_{\text{CDW}}|$ favors the coupling of momenta, which are rather distant from each other, thus reducing the effect of the anisotropic density of states. Consequently, the gap anisotropy is smeared and also in this case the lines of nodes of the *d*-wave solution are made comparatively less favorable. Notice also that this latter effect is more pronounced for the instability in the (1,1) direction because the phase of the order parameter in the *d*-wave superconductivity is hardly compatible with an attractive potential strongly scattering states close to the $(\pi, 0)$ - $(0, \pi)$ points of the Brillouin zone.⁵⁵

We finally like to point out that fixing $\langle V_{\text{attr}}(q_x, q_y) \rangle$ in order to obtain (for the pure *d* wave) a critical temperature around 100 K, in all cases U^* turns out to be quite small (a few hundreds of eV).

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