Possible secondary component of the order parameter observed in London penetration depth measurements

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We discuss the effect of a secondary component of the superconducting order parameter on the superfluid density in the cuprates. If we assume a main $d_{x^2-y^2}$ gap, the most stable realization of a mixed order parameter has a time-reversal breaking $d_{x^2-y^2}+\imath d_{xy}$ symmetry. In this state the nodes are removed and the temperature dependence of the superfluid density changes from the linear behavior of a pure d wave to a more rounded shape at low temperature. The latter is compatible with the behavior experimentally observed in the in-plane magnetic field penetration depth of optimally doped $La_{2-x}Sr_xCuO_2$ and $YBa_2Cu_3O_{7-y}$.

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I. INTRODUCTION

The identification of the pairing mechanism behind high-temperature superconductivity in copper oxides[1] remains one of the greatest challenges in solid state physics. A key ingredient is the symmetry of the order parameter, which is expected to reflect that of the pairing interaction thus providing information on the microscopic mechanism. The well-established evidence of lines with vanishing amplitude in the gap function of cuprates along the Γ-X direction of the Brillouin zone (nodes) indicates a dominant $d_{x^2-y^2}$ symmetry of the order parameter,[2] hardly compatible with the standard phonon pairing mechanism, which leads to an isotropic s-wave order parameter. Anyway a small secondary component of the order parameter can develop either spontaneously or driven by external factors such as magnetic field, doping or presence of magnetic impurities.[3–5] The development of a mixed order parameter has been also invoked to explain anomalies observed in the thermal conductivity in magnetic field of $Bi_2Sr_2CaCu_2O_8$.[6] Moreover substantial deviation from the $d_{x^2-y^2}$-wave symmetry has been observed in $YBa_2Cu_3O_{7-y}$ (YBCO) both in tunneling measurements[7] and in laser angle-resolved photoemission revealing nodeless bulk superconductivity.[8] A series of low-temperatures anomalies has been observed in the in-plane magnetic field penetration depth in muon-spin rotation (μSR) experiments.[9–12] Experiments in optimally doped $La_{2-x}Sr_xCuO_2$ (LSCO) (Ref. 9) and YBCO (Refs. 10 and 12) have shown a low-temperature bump in the penetration depth superimposed to the linear temperature behavior associated to d-wave superconductivity and to the presence of nodes. These deviations from d-wave behavior have been associated to a secondary component, which has been proposed to be isotropic s wave in light of its vulnerability to a magnetic field.[9,10,13] Alternative proposals[14,15] do not assume the presence of a mixed order parameter and they associate the low-temperature feature either to a nonlocal response of the d-wave superconductor, which modifies the magnetic field distribution in the vortex state with respect to the standard London model or to a particle-hole secondary gap associated to spin-density wave ordering.[16]

Here we focus on the secondary superconducting gap interpretation, and we show that a $d_{x^2-y^2}+\imath d_{xy}$ mixed order parameter can reasonably describe the μSR experimental results. Under rather general assumptions, a previous analysis[17] has shown that, once a leading $d_{x^2-y^2}$ symmetry is assumed, this time-reversal breaking $d_{x^2-y^2}+\imath d_{xy}$ symmetry is the most stable realization of a mixed order parameter.

This work is organized as follows. In Sec. II we present our model and approach. In Sec. III we discuss the general behavior of the superfluid density with a mixed order parameter and presents the comparison with experiments. Section IV contains our conclusions.

II. MODEL

In this section we briefly summarize the formalism used in Ref. 17 to identify the conditions for a secondary component to establish in the presence of a dominant $d_{x^2-y^2}$ wave. We consider a two-dimensional square lattice characterized by the $\mathcal{C}_{4v}$ point group and a single band with dispersion

$$\xi_{\mathbf{k}} = -2t(\cos \mathbf{k}_x a - \cos \mathbf{k}_y a) + 4t' \cos \mathbf{k}_x a \cos \mathbf{k}_y a - \mu, \tag{1}$$

where t and t' are the nearest and next-nearest hopping parameters, μ is the chemical potential and $a=1$ is the lattice spacing. Values of t and t' for different compounds have been chosen according to density-functional theory calculations in the local-density approximation.[18]

The aim of the present analysis is the understanding of the competition between the different components of a superconducting order parameter. Therefore we do not attempt a solution of a microscopic model including different kind of realistic interactions, and we simply consider an effective low-energy interaction, whose strength in each symmetry channel controls the corresponding instability. Moreover, we will study the superconducting phase within the Bardeen-Cooper-Schrieffer (BCS) mean-field approach, which fully takes into account for the symmetry of the order parameter. This approach is reasonably justified for instance by the relatively large doping of the samples of Refs. 9, 10, and 12

We now briefly recall some relevant aspects of the BCS equations for a mixed order parameter, referring to Ref. 17 and references therein for more details. If we require the invariance under the symmetry of the lattice of the modulus of the order parameter, the latter has to transform either as an irreducible representation or as a complex combination of the form $\Delta^{\mu}+\imath\Delta^{\nu}$ (with Δ^{μ} and Δ^{ν} transforming as two different irreducible representations) which breaks time-reversal invariance. The development of each harmonic with a given symmetry is controlled by a specific spatial component of the pair potential. The isotropic s wave is associated to the local component of the potential V_0, the $d_{x^2-y^2}$ and extended-s ($s_{x^2+y^2}$) are controlled by the nearest-neighbor coupling V_1 while the d_{xy} and s_{xy} (which are analogous to $d_{x^2-y^2}$ and $s_{x^2+y^2}$ with lobes along the diagonal directions in the plane) are related to the next-neighbor coupling V_2. Here we will simply assume that V_0 is repulsive due to the local Coulomb repulsion and that V_1 and V_2 are attractive. For the sake of definiteness we report the equations for the $d_{x^2-y^2}+\imath d_{xy}$ mixed order parameter

$$\begin{cases} \dfrac{1}{V_1} = -\sum_{\mathbf{k}} \omega_d^2(\mathbf{k}) \dfrac{1}{2\epsilon_{\mathbf{k}}} \tanh\left(\dfrac{1}{2}\beta\epsilon_{\mathbf{k}}\right) \\ \dfrac{1}{V_2} = -\sum_{\mathbf{k}} \omega_{d'}^2(\mathbf{k}) \dfrac{1}{2\epsilon_{\mathbf{k}}} \tanh\left(\dfrac{1}{2}\beta\epsilon_{\mathbf{k}}\right) \\ n = 1 - \sum_{\mathbf{k}} \dfrac{\xi_{\mathbf{k}}}{\epsilon_{\mathbf{k}}} \tanh\left(\dfrac{1}{2}\beta\epsilon_{\mathbf{k}}\right). \end{cases} \quad (2)$$

Here $\beta=1/T$ is the inverse temperature, $\omega_d(\mathbf{k})=\cos(\mathbf{k}_x a)-\cos(\mathbf{k}_y a)$ and $\omega_{d'}(\mathbf{k})=2\sin(\mathbf{k}_x a)\sin(\mathbf{k}_y a)$ are the harmonics associated to $d_{x^2-y^2}$ and d_{xy} wave, respectively, Δ_d and $\Delta_{d'}$ are the associated components of the gap and $\epsilon_{\mathbf{k}}=\sqrt{\xi_{\mathbf{k}}^2+\Delta_d^2\omega_d^2(\mathbf{k})+\Delta_{d'}^2\omega_{d'}^2(\mathbf{k})}$. The superconducting gaps Δ_d, $\Delta_{d'}$ and the chemical potential μ are derived solving self-consistently Eqs. (2). An energy cutoff ω_0 is used in the first two k sums.

For realistic dispersions, the $d_{x^2-y^2}$ symmetry is the leading instability. When the main $d_{x^2-y^2}$ order parameter appears at T_c, for $T<T_c$ the effective dispersion $\epsilon_{\mathbf{k}}$ is gapped and any secondary instability requires a minimum (critical) value for the associated interaction strength, as opposed to the case of an instability developing in a Fermi sea. The d_{xy} component turns out to be the best candidate for the secondary gap (i.e., it has the lowest critical value of the interaction) since it has the largest contributions from the regions in which the main gap has nodes. Since the onset of a secondary component is essentially determined by the competition with the main gap, one can favor a mixed state by reducing the $d_{x^2-y^2}$ component. The complementarity between d_{xy} and $d_{x^2-y^2}$ also implies that the two components can exist simultaneously for a wide range of parameters. A secondary order parameter with a different symmetry can instead less efficiently exploit the Fermi-surface portions in which the first gap has nodes. Therefore, if we increase the associated coupling, we have an abrupt change from a pure $d_{x^2-y^2}$ to a pure order parameter of different symmetry, and a very fine tuning is required to have both order parameters. This is the case of a $d_{x^2-y^2}+is_{xy}$, which has the second smallest critical coupling but it rapidly turns into a pure s_{xy} as V_2 is further increased. For example, using $V_1=230$ meV, $t=200$ meV, $t'/t=0.25$ the critical V_2 for the is_{xy} component is 1.15 times that of the id_{xy} gap but the mixed order parameter only exists in a tiny 0.02 meV window, and it is rapidly replaced by a pure s_{xy} wave which is not relevant to experiments.

The focus of this paper is the effect of a secondary component of the superconducting order parameter on the superfluid density ρ_s, which is directly related to the London penetration depth by the relation $\lambda^{-2}=4\pi e^2\rho_s/mc^2$, being m the electron mass and c the speed of light. ρ_s is defined as

$$\rho_s = \sum_{\sigma} \frac{\partial^2 \xi_{\mathbf{k}}}{\partial \mathbf{k}^2}\langle c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma}\rangle - \lim_{k\to 0}\int_0^{\beta} d\tau \langle j(\mathbf{k}\tau) j(-\mathbf{k}0)\rangle, \quad (3)$$

where the first term is the zero-temperature contribution while the other is the current-current response. For BCS pairing, in case of spin degeneracy, the previous expression then reads

$$\rho_s = \sum_{\mathbf{k}} \frac{\partial^2 \xi_{\mathbf{k}}}{\partial \mathbf{k}^2}\left[1 - \frac{\xi_{\mathbf{k}}}{\epsilon_{\mathbf{k}}}\tanh\left(\frac{\beta\epsilon_{\mathbf{k}}}{2}\right)\right] + 2\sum_{\mathbf{k}}\left(\frac{\partial \xi_{\mathbf{k}}}{\partial \mathbf{k}}\right)^2 \frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}} \quad (4)$$

being $f(\epsilon_{\mathbf{k}})=1/(e^{\beta\epsilon_{\mathbf{k}}}+1)$ the Fermi-distribution function for the Bogoliubov quasiparticles.

III. SUPERFLUID DENSITY IN THE MIXED STATE

Before addressing the comparison with experimental data, we consider the effect of the onset of the $d_{x^2-y^2}+id_{xy}$ mixed order parameter in general terms. In Fig. 1(a) we plot the temperature dependence of the superfluid density and of the components of the superconducting gap, normalized to their $T=0$ values (the parameters are reported in the figure caption). Indeed the results show that the linear temperature behavior characteristic of the d-wave state,[16] associated to the presence of nodal quasi particles, is modified below a temperature T_c' [see Fig. 1(a)]. The low-temperature feature of the superfluid density is clearly related to the development of a d_{xy} gap, which fills the nodes of the $d_{x^2-y^2}$ component below the secondary "critical temperature" T_c'. In this regime, in which a $d_{x^2-y^2}+\imath d_{xy}$ order parameter is stable, the shape of the superfluid density is more similar to that of a usual s-wave superconductor, reflecting the absence of low-energy excitations. This shows that an "s-wavelike" behavior at low temperatures does not automatically suggest an s-wave component and that the $d_{x^2-y^2}+id_{xy}$ order parameter generates a temperature behavior which reproduces the qualitative results of Refs. 9, 10, and 12.

We now briefly discuss how the shape of the superfluid density depends the parameters of the system. A crucial parameter which varies in the different cuprates is the next-neighbor hopping t' (Ref. 18) which controls the position of the Van Hove singularity (VHS).[19] Therefore t' can push the singularity close to the chemical potential, thereby favoring the $d_{x^2-y^2}$ at the expenses of the secondary gap. Indeed, as

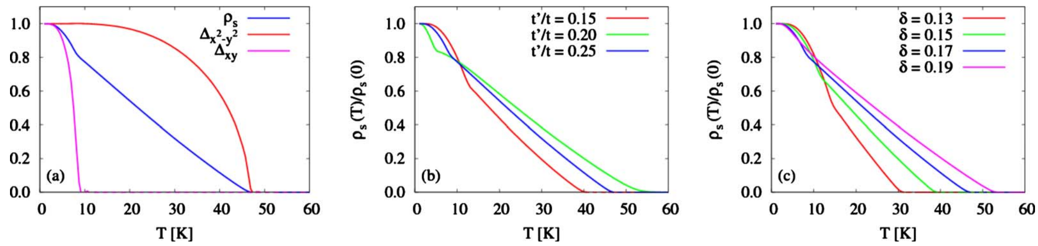

FIG. 1. (Color online) (a) Typical behavior of ρ_s and superconducting gaps $\Delta_{x^2-y^2}$ and Δ_{xy} as a function of T. The parameters are $t=200$ meV, $V_1/t=0.50$, $V_2/t=1.00$, $\omega_0/t=0.25$, $t'/t=0.25$, and doping $\delta=0.17$. Each quantity has been normalized to its $T=0$ value in order to better compare the curves. The low-energy feature is associated to the opening of the secondary gap. (b) Behavior of ρ_s for different values of t'/t and $\delta=0.17$, and (c) Behavior of ρ_s for different dopings and $t'/t=0.25$. [In panels (b) and (c) t, V_1, V_2, and ω_0 are as in panel (a).]

shown in Fig. 1(b) at fixed doping T_c' decreases as the chemical potential approaches the VHS. The same behavior holds for the amplitude of the secondary gap as expected within BCS. Similar results are naturally obtained by changing the hole concentration instead of t' [see Fig. 1(c)], i.e., changing the chemical potential and its position with respect to the VHS. In practice the variation in t' in different materials can be quite large, and it affects the symmetry of the order parameter much more than doping variations within the physically relevant regime. In some cases [e.g., in LSCO compounds, where $t'/t \simeq 0.15$ (Ref. 18)], the chemical potential can approach or cross the VHS in the relevant doping range. On the other hand when t' is larger (e.g., in YBCO compounds) and the singularity is far from the Fermi level, the effect of doping becomes less important. Also orthorhombic distortions or bilayer splitting reduce the $d_{x^2-y^2}$ gap, allowing for a larger secondary component.[17] As a more technical note, the value of the cutoff ω_0 plays a role in the stability of the secondary component because it selects the portion of density of states which contributes to the effective coupling, i.e., a small cutoff makes the system more sensitive to the details of the bandstructure.[20] For the range of parameters of interest this reflects in a stronger effect of the VHS, which favors the main component at the expenses of the secondary one.

We now turn to the experimental evidences discussed above considering the specific cases of optimally doped LSCO (Ref. 9) and YBCO.[12] We use parameters ($t=200$ meV and $V_1=0.55t$, $V_2=1.10t$, $\omega_0=0.25t$, $t'=0.135t$ for LSCO and $V_1=1.10t$, $V_2=1.275t$, $\omega_0=0.25t$, $t'=0.35t$ for YBCO) that reproduce the experimental dispersions and the zero-temperature value of the gaps. The doping is $\delta \equiv 1-n=0.17$ in both cases. As shown in Fig. 2, our simple theoretical approach well reproduces the temperature behavior of ρ_s for a wide range of temperature. The appearance of the secondary component is much more pronounced for LSCO, in agreement with the above analysis about the role of t'/t. The deviation between the BCS results and the experiments close to T_c are obviously expected because of the relevance of fluctuations for quasi two-dimensional strong-coupling superconductors.

Our analysis shows that the experimental evidence of a low-temperature "bump" on top of the linear temperature dependence can be understood in terms of a $d_{x^2-y^2}+id_{xy}$ order parameter without invoking an s-wave component. In our calculations we can get an isotropic s-wave component only if we relax the assumption of a repulsive V_0. In this case we obtain a mixed $d_{x^2-y^2}+is$ for a sizeable local attraction V_0. This is hardly compatible with the strong local repulsion responsible of the Mott state in cuprates.

As a final remark we focus our attention on the effect of an external magnetic field, which seems to flatten out the low-temperature behavior of the penetration depth in the experimental data.[9,10] Several conflicting interpretations have been proposed. Some of them[14,16] relate the flattening to a nonlocal response of the d-wave superconductor. Other studies identify the low-temperature feature with a second gap being either spin-density wave[15] or a different superconducting gap in the same spirit of the present analysis.[13] In Ref.

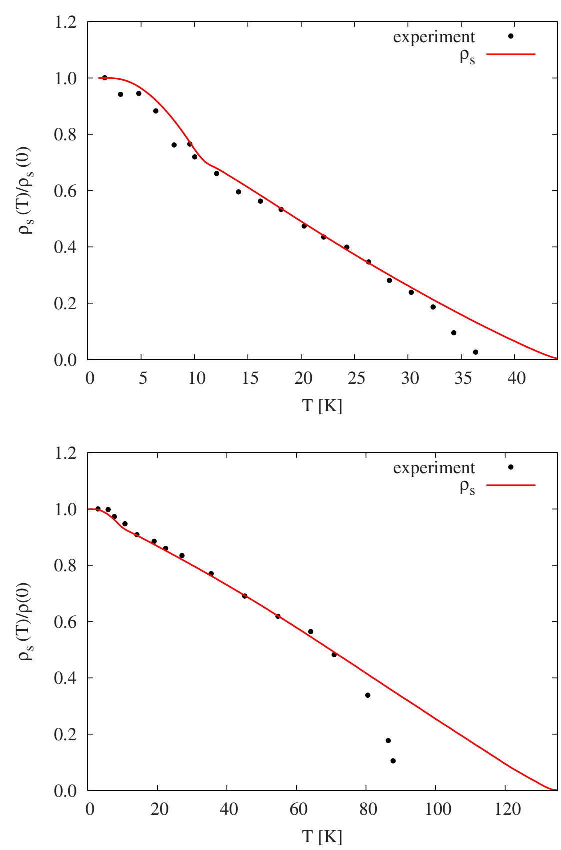

FIG. 2. (Color online) Theoretical results for superfluid density against experimental data for the (normalized) spin depolarization rate on $La_{1.83}Sr_{0.17}CuO_4$ (Ref. 9) and $YBa_2Cu_3O_{6.95}$ (Ref. 12) compounds.

13, in particular, the fragility of the secondary component to an external magnetic field has been advocated as a proof of its *s*-wave nature. It is crucial to observe that the experimental magnetic fields (0.02, 0.1, and 0.64 T) (Ref. 9) are too low to directly affect the secondary gap, whatever the mechanism could be. In this sense, the effect of these small fields can only be a minor indirect consequence, and it hardly shed lights on the symmetry of the secondary component. Within the second gap interpretation, we notice that the main element for the stability of the secondary component is actually the size of the main gap, and that tiny variations in the latter may completely suppress the former.

IV. CONCLUSIONS

In this paper we have analyzed the effect of a time-reversal breaking order parameter $d_{x^2-y^2}+id_{xy}$ on the temperature evolution of the superfluid density within a BCS formalism. This combination turns out to be the most stable mixed order parameter if the main component has $d_{x^2-y^2}$ symmetry.[17] Moreover, as opposed to the anisotropic is_{xy} component, it allows for a smooth evolution from a pure *d* wave to a superconducting phase which displays a secondary component at low temperature. The same smooth evolution is mirrored in the temperature behavior of the superfluid density, in which a small bump is superimposed to the linear behavior characteristic of a pure $d_{x^2-y^2}$ wave.

We compared numerical results to experimental data on two cuprates and showed that the low-temperature feature observed in μSR measurements can be reproduced assuming reasonable parameters for the system in such an unconventional symmetry phase.

Our calculations show that the opening of a secondary gap requires a fine tuning of the parameters. Therefore more experimental confirmations are needed to assess this secondary order parameter as an intrinsic property of the cuprates.

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