Effect of magnetic field on the competition between superconductivity and charge order below the pseudogap state

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We theoretically investigate the T-B phase diagram of cuprates building on the SU(2) pseudogap order recently obtained from the spin-fermion model. At low temperatures, our analysis reveals an almost temperature-independent critical magnetic field B_{co} at which d-wave superconductivity switches to a phase of charge order. For temperatures beyond a certain value of the order of the zero-field superconducting transition temperature T_c , the critical field $B_{co}(T)$ sharply grows. We compare our results derived within the effective SU(2) nonlinear σ model with the phase diagram recently obtained by sound velocity measurements by LeBoeuf $et\ al.$ [Nat. Phys. 9, 79 (2013)].

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I. OVERVIEW

After more than 25 years of investigation, high- T_c cuprate superconductors still retain much of their mystery. At the same time, experiments quarried a huge body of unprecedented data to fuel the theoretical investigation. Among all the phases these compounds exhibit, the normal phase and especially the infamous "pseudogap" phase remain particularly controversial. The proximity to antiferromagnetism, the vicinity of a metal-insulator Mott transition, preformed superconducting pairs, or the presence of hidden competing orders are exemplary scenarios that have been suggested to explain the curious depression in most thermodynamic and transport quantities within the pseudogap. 2

Recently, a series of ground-breaking experiments has revived the debate about the presence of a modulated state in competition with superconductivity. While in Labased superconductors the presence of static modulated spin-charge orders at commensurate doping close to 1/8 is now well established,³ the situation for YBa₂Cu₃O_{6+x} and $Bi_2Sr_2CaCu_2O_{8+\delta}$ compounds is much less clear. First, if we assume a stripe order, it is most probably of a dynamical nature in these compounds, and second, it has been suggested that the modulation in those compounds is biaxial, of the form of a checkerboard, as reported by scanning tunneling microscopies (STM) in $Bi_2Sr_2CaCu_2O_{8+\delta}$. In contrast to the stripe structure, the checkerboard structure has been claimed to be incommensurate with the Cu-O lattice, with a periodicity determined by wave vectors close to those connecting the nearest antinodes.

Soft^{6,7} and hard x-ray^{8,9} measurements confirmed these findings, disclosing the presence of an incommensurable biaxial purely charge structure in YBa₂Cu₃O_{6+x} in the doping range $0.09 \leqslant p \leqslant 0.13$, with modulation wave vectors compatible with those observed by STM. Quantum oscillation measurements^{10,11} associated with a negative Seebeck coefficient and negative Hall constant point out the existence of at least one small electron pocket at low temperatures. ^{12–15} The Fermi surface reconstruction implied by these measurements may be attributed to the proximity of a competing modulated order. This interpretation is in line with the results of earlier nuclear magnetic resonance (NMR) measurements, ^{16,17}

indicating the existence of a modulated charge order, though not being decisive yet about whether the form is stripes or checkerboard and commensurate or incommensurate.

The charge order observed in these experiments appears or is enhanced under the application of an external magnetic field $B.^{8,16,18}$ A recent study 18 of the T-B phase diagram of underdoped YBa $_2$ Cu $_3$ O $_{6+x}$ with p=0.108 has revealed interesting features and convincing evidence for a two-dimensional charge modulation. Applying magnetic fields up to 30 T, the authors of Ref. 18 extracted from ultrasound measurements the elastic constants of the compound, which allowed to identify the phase transitions. Below a critical temperature $T_{\rm co} \approx 40$ K, a static charge order stabilizes abruptly above a critical field of $B_{\rm co} \approx 18$ T that is temperature independent (see Fig. 2 of Ref. 18). Contrarily, for magnetic fields $B > B_{\rm co}$, the boundary of the static charge order practically remains of order $T_{\rm co}$, only weakly depending on the magnetic field.

In a recent theoretical work¹⁹ on the antiferromagnetnormal metal quantum critical point (QCP), several of us have come to a conclusion about the existence of a pseudogap phase in its vicinity that is characterized by a composite SU(2)order parameter, combining the d-wave superconducting and a particle-hole suborder. The latter is a charge order characterized by a spatially modulated electric quadrupolar moment and may thus be referred to as a quadrupole density wave. The degeneracy between superconductivity and charge order is lifted for a finite Fermi surface curvature, resulting in the stabilization of superconductivity at low temperatures T < T_c . At higher temperatures $T_c < T < T^*$ —the pseudogap region—thermal fluctuations described by an SU(2) nonlinear σ model are strong and prevent the two suborders from disentangling. Here, they are mixed together but fluctuations destroy any long-range order.

In this Rapid Communication, we generalize the nonlinear σ model derived in Ref. 19 and include an external magnetic field B affecting the orbital motion. As the electron pairing is purely singlet, effects of the magnetic field on the electron spins are negligible. The magnetic field B favors the charge suborder of the pseudogap. Sufficiently strong fields $B > B_0$ may even surmount the curvature threshold and establish a charge order at low temperatures. The system is thus allowed

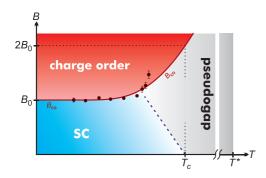


FIG. 1. (Color online) T-B phase diagram following our analysis of the fluctuations around the mean-field order parameter of the spin-fermion model. The dark red dots are from the sound velocity measurements reported in Ref. 18 with $B_0 \approx 18$ T and $T_c \approx 60.7$ K while the red curve $B_{\rm co}(T)$, Eq. (14), has been fitted to the experimental data with the constraint that $B_{\rm co}(T_c) = 2B_0$.

to switch between the two suborders, superconductivity and charge order, which is controlled by the strength of the applied field. At the critical field B_0 , the system is degenerate between superconducting and particle-hole order states. The fact that such a simple switching mechanism might be at the heart of the physics of the pseudogap state in the cuprates is very interesting and may even have the potential to restrain the window of validity of theoretical interpretations.

Our main results are illustrated by Fig. 1 representing in the T-B plane the regions of charge order, d-wave superconductivity (SC), and the pseudogap state. We see that the border between the charge order and the SC state is flat at low temperatures while the charge order—and SC—pseudogap borders depend on the magnetic field B only logarithmically. This picture agrees well with the experimental T-B phase diagram of Ref. 18.

II. MODEL FOR THE PSEUDOGAP STATE

We investigate the pseudogap state in the cuprate superconductors beginning with an effective spin-fermion model (see, e.g., Refs. 20 and 21) describing electrons coupled to quantum critical antiferromagnetic paramagnons. The Lagrangian for the (2+1)-dimensional model is written as

$$\mathcal{L} = \chi^{\dagger} (\hbar \partial_{\tau} + \varepsilon (-i\hbar \nabla) + \lambda \vec{\phi} \vec{\sigma}) \chi. \tag{1}$$

The field $\vec{\phi}$ describes the paramagnons that couple to the spin $\vec{\sigma}$ of the electronic fields χ . The paramagnon excitations are modeled by the correlation function

$$\langle \phi_{\omega,\mathbf{k}}^i \phi_{-\omega,-\mathbf{k}}^j \rangle \propto \frac{\delta_{ij}}{(\omega/v_s)^2 + (\mathbf{k} - \mathbf{Q})^2 + a},$$
 (2)

where v_s is the wave velocity and \mathbf{Q} the antiferromagnetic ordering vector below the QCP. The distance to the QCP is controlled by the parameter a with the QCP itself situated at a=0. In this study, we consider the proximity of the QCP to its right ($a \ge 0$) but, at finite temperatures, the results should also apply qualitatively to the near quantum critical region on its left (a < 0). Landau damping modifies the paramagnon propagator but this effect is reduced when the pseudogap opens. ¹⁹

The mean-field analysis¹⁹ of the spin-fermion model (1) indicates that below a temperature T^* , orders in both

the superconducting and particle-hole channel emerge and combine to form a composite order parameter $O(\varepsilon) = b(\varepsilon)u$, with $b(\varepsilon)$ a function of fermionic Matsubara frequencies and u denoting an SU(2) matrix in the Gor'kov-Nambu particle-hole space. The typical scale of $b(\varepsilon)$ is k_BT^* . The matrix u can be parametrized by two complex order parameters Δ_+ and Δ_- for superconducting and charge suborders, respectively,

$$u = \begin{pmatrix} \Delta_{-} & \Delta_{+} \\ -\Delta_{+}^{*} & \Delta_{-}^{*} \end{pmatrix} \tag{3}$$

while unitarity imposes the constraint $|\Delta_+|^2 + |\Delta_-|^2 = 1$.

As shown in Ref. 19, fluctuations around a particular mean-field solution are accurately described in terms of a two-dimensional SU(2) nonlinear σ model. At temperatures T > 0, the partition function for the low-lying Goldstone modes has the form $\mathcal{Z} = \int \exp(-\mathcal{F})\mathcal{D}u$, with

$$\mathcal{F} = \frac{1}{t} \int \text{tr}[\nabla u^{\dagger} \nabla u + \kappa^2 u^{\dagger} \tau_3 u \tau_3] d^2 \mathbf{r}. \tag{4}$$

In terms of microscopic parameters, $t=(8\pi/J_1\sin\delta)(k_BT/\hbar vS)$, where v is the Fermi velocity, S the size of a gapped hot spot on the Fermi surface, and δ the angle between the Fermi velocities at two hot spots connected by the ordering vector $\mathbf{Q}.^{22}$ For $T < T^*$, $J_1 \sim \bar{J}_1 \approx 0.25$, whereas approaching T^* , J_1 turns to zero (cf. the Supplemental Material of Ref. 19). We may estimate T^* by $k_BT^* = \alpha^{-1}(2\bar{J}_1\sin\delta/3)\hbar vS$ with $\alpha \sim 1$. The coupling constant $t = (16\pi/3)(T/\alpha T^*)$ is the effective temperature in the σ model.

The coupling constant κ^2 of the second term in Eq. (4) emerges from curvature corrections to the linearized spin-fermion model. On the right of the QCP, κ^2 is enhanced with growing a>0. Containing the third Pauli matrix τ_3 in the Gor'kov-Nambu space, the second term breaks the SU(2) rotational symmetry between the particle-hole and superconducting suborders to favor the latter. The renormalization group (RG) analysis shows that superconductivity is stabilized below a temperature $T_c < T^*$ determined by the magnitude of κ . The transition between superconductivity and the disordered pseudogap phase is driven by thermal fluctuations. The SU(2) symmetry of the linearized spin-fermion model has first been noticed in Ref. 21, where the particle-hole order was discussed as a subleading instability in the bond correlation functions.

In order to investigate the T-B phase diagram, we insert the magnetic field B into the nonlinear σ model (4) by making the replacement

$$\nabla u \to \nabla u + ie\bar{\mathbf{A}}[\tau_3, u],$$
 (5)

where $[\cdot,\cdot]$ is the commutator. In Landau gauge, $\bar{\mathbf{A}}(x,y) = -\frac{1}{2}\sin\delta By\mathbf{e}_x$, with \mathbf{e}_x the unit vector in the x direction. The unusual prefactor of $\frac{1}{2}\sin\delta$ in the "reduced vector potential" $\bar{\mathbf{A}}$ is due to a change of coordinates during the derivation of Eq. (4) (cf. Ref. 19).

III. T-B PHASE DIAGRAM

Charge order–SC transition. Let us first consider the transition between superconductivity (SC) and the charge suborder at low temperatures $T \ll T^*$. The critical field $B_{\rm co}$ of this transition is at the same time the field $B_{\rm c2}$ of the type-II

superconductor. At very strong magnetic fields, SC clearly may not exist so that the charge order prevails instead. In order to look for the first appearance of the superconducting order parameter when lowering the magnetic field B, we may assume that $|\Delta_+|$ [cf. Eq. (3)] is small and expand the functional \mathcal{F} for the free energy up to quadratic terms in Δ_+ ,

$$\mathcal{F}[\Delta_{+},\chi] \simeq \frac{1}{t} \int \{ |(\nabla + 2ie\bar{\mathbf{A}})\Delta_{+}|^{2} - 2\kappa^{2}|\Delta_{+}|^{2} + (\nabla \chi)^{2}(1 - |\Delta_{+}|^{2}) \} d^{2}\mathbf{r}, \tag{6}$$

with χ the phase of the charge order parameter Δ_- .

This quadratic form is strictly positive in the charge order state but loses its stability at $B < B_{\rm co}$. At low temperatures, we can neglect the $(\nabla \chi)^2$ term. Then the study of the approximated functional in Eq. (6) is reduced to solving the Schrödinger equation in the presence of a magnetic field. As a result, we find that nonzero solutions for Δ_+ appear below the critical magnetic field $B_{\rm co} = B_0$ with

$$B_0 = \frac{\hbar \kappa^2}{e \sin \delta}.\tag{7}$$

Below B_0 , we expect the formation of superconducting vortices that in contrast to the usual scenario must contain charge order cores instead of normal metal phases. The details of the physics in this region of the phase diagram and, in particular, the question of coexistence of charge and superconducting orders at low temperatures 17,23 will be left for a separate study.

Equation (7) shows that at small T, where thermal fluctuations are weak, the critical field $B_{\rm co}$ does not depend on temperature. It also relates the value of the coupling constant κ^2 of the σ model (4) to the experimentally measurable magnetic field B_0 that separates the two phases.

SC-pseudogap and charge order–pseudogap transitions. In the absence of a magnetic field, superconductivity is stabilized at temperatures $T < T_c$, whereas at $T > T_c$ thermal fluctuations destroy a long-range order in the pseudogap. If, due to a strong magnetic field, the ground state is a charge order, we may expect a similar transition between pseudogap and this order, which is stabilized up to a critical temperature T_{co} .

In the absence of a magnetic field, these fluctuations have been studied in the superconducting phase using the renormalization group (RG) method.¹⁹ Integrating out step by step the fast fluctuations around the mean-field solution $u=i\tau_2$ for superconductivity, we reproduce the free energy functional $\mathcal F$ while the coupling constants flow according to the RG equations

$$\frac{dt}{d\xi} = \frac{3}{16\pi}t^2, \quad \frac{d\ln(\kappa^2/t)}{d\xi} = -\frac{3}{8\pi}t,$$
(8)

where ξ is the running logarithmic variable of the RG (see the Supplemental Material to Ref. 19).

Equations (8) lead to a solution for t increasing with ξ and one for κ that decreases. The RG flow stops at $\xi = \ln(l_{\min}^{-1}/\kappa)$, yielding

$$t = t_b \left[1 + \frac{3t_b}{16\pi} \ln\left(l_{\min}\kappa\right) \right]^{-1},\tag{9}$$

$$\kappa^2 = \kappa_b^2 \left[1 + \frac{3t_b}{16\pi} \ln(l_{\min}\kappa) \right]. \tag{10}$$

The ultraviolet cutoff in the logarithms is $l_{\min} \propto \lambda^{-2}$, the minimal length in the theory. The parameters t_b and κ_b^2 denote the bare coupling constants, determined by the actual values of temperature and curvature of the system. The coupling constant κ_b^2 constitutes a gap in the excitation spectrum.

At small κ , the effective temperature t becomes large, which should be interpreted as a phase transition from superconductivity to the disordered pseudogap. Since simultaneously the effective anisotropy κ vanishes, charge and SC suborders are equally distributed in the pseudogap without a long-range order being formed. The coupling constant t diverges at the temperature

$$T_c = \alpha T^* \frac{1}{\ln\left(l_{\min}^{-1}/\kappa_b\right)},\tag{11}$$

where $\alpha \sim 1$ [cf. the paragraph after Eq. (4)]. The transition temperature T_c can thus be considerably lower than T^* where the pseudogap turns into the normal state.

In the presence of an external magnetic field, the critical temperature T_c , Eq. (11), does not change as long as the system remains in the Meissner state ($B < B_{c1}$). For $B > B_{c1}$, vortices penetrate the sample, the ground state is no longer homogeneous, and RG studies are more difficult.

At the same time, the RG scheme presented above is applicable to the charge order–pseudogap transition since the ground state for $B > B_0$ [see Eq. (7)] is also homogeneous. However, as easily seen [cf. Eq. (6)], the gap in the excitation spectrum is now given by $\ell_B^{-2} - \kappa^2$, where

$$\ell_B = \sqrt{\frac{\hbar}{eB\sin\delta}} \gg l_{\min} \tag{12}$$

is the magnetic length. For the charge order state, we study fluctuations around the mean-field solution u=1, yielding the same RG equations (8) and the same solutions (9) and (10), yet the coupling constant κ^2 has to be replaced by the gap $\ell_B^{-2} - \kappa^2$ that we treat as an effective coupling constant. As a result, we come to the charge order–pseudogap transition temperature

$$T_{co}(B) = \alpha T^* \frac{1}{\ln\left[l_{\min}^{-1}/(\ell_B^{-2} - \kappa^2)^{1/2}\right]}.$$
 (13)

For not too large magnetic fields $B < 2B_0$, $T_{\rm co}$ is smaller than the superconducting transition temperature T_c , Eq. (11), while at $B = 2B_0$, we have $T_{\rm co}(2B_0) = T_c$. At larger B, $T_{\rm co}$ grows slowly and the charge order–pseudogap critical line in the T-B plane appears practically vertical. Formula (13) actually is applicable down to the critical field B_0 , Eq. (7). Rewriting Eq. (13) as

$$B_{\rm co} = B_0 \left(1 + \frac{1}{l_{\rm min}^2 \kappa_b^2} \exp\left\{ -\frac{2\alpha T^*}{T} \right\} \right) \tag{14}$$

yields a formula for the critical curve $B_{co}(T)$ valid for all temperatures and the horizontal line in the T-B plane at low T is evident. On this line, the physics is characterized by degeneracy between the two suborders just as in the pseudogap at larger T.

Phase diagram. Equation (14) leads to the T-B phase diagram in Fig. 1. The boundary separating the SC and charge order phases is determined by the asymptotic limit (7) and is

flat up to temperatures $\sim T_c$, Eq. (11). The pseudogap state, characterized by the absence of charge or SC long-range orders, is located to the right of the phase boundaries of the ordered regions, but charge and SC suborders are as well equally distributed on the critical line separating them. The SC critical temperature T_c at zero field agrees with the transition temperature T_{co} at $B=2B_0$. Finally, the transition between SC and pseudogap at a finite magnetic field $B < B_0$ is qualitatively indicated by the dashed line in Fig. 1, which also determines B_{c2} .

IV. COMPARISON WITH EXPERIMENTS

Our conclusions agree with results of the recent experimental work ¹⁸ by LeBoeuf *et al.* Measuring sound velocities in underdoped YBa₂Cu₃O_y in various directions up to magnetic fields of 30 T, the authors encountered a thermodynamic transition between superconductivity and a different state characterized by a biaxial charge order. Referring to earlier NMR measurements, ¹⁶ they attributed this state to a "static charge" order.

Following our results, we identify the critical magnetic field $B_{\rm co}$ of Ref. 18 with the field $B_{\rm co}$ of Eq. (14). Specifically at temperatures below $T_{\rm co}\approx 40$ K, the field $B_{\rm co}$ was reported to be almost flat at $B_{\rm co}\approx 18$ T. This corresponds to our theoretical low-temperature behavior (cf. Fig. 1). The right boundary of the charge order grows fast experimentally, which also is reflected in and explained by the phase diagram and Eq. (14) of our analysis. We mention that the transition to charge ordering at $B\approx 28.5$ T and $T=(50\pm 10)$ K as detected by NMR¹⁶ agrees with our theoretical phase diagram as well. Furthermore, the interpretation of the data in terms of the biaxial charge order supports the theoretical prediction¹⁹ of a checkerboard modulation.

Previous studies on the competition between superconductivity and another order were typically based on Ginzburg-Landau-type (GL) theories with the competing state typically chosen to be a spin-density wave (SDW) (see, e.g., Refs. 24–26). In such approaches, however, it is not easy to explain the flat lower boundary of the "static charge" order in Fig. 2 of Ref. 18 because in GL theories the upper critical field B_{c2} , which should agree with this boundary, essentially depends on temperature. Moreover, GL theories

lack the emergence of the pseudogap state, and the prediction of SDW competing with SC does not fit the experimental evidence. Finally, we mention that the competition between superconductivity and a charge order has also been studied in phenomenological models assuming interactions mediated by nearly critical charge collective modes.

It is useful to extract numerical estimates for the coupling constants in the model (4) using the experimental data. By Eq. (7), the experimental value $B_0 \approx 18$ T yields under the assumption $\sin \delta = 0.5$ that $\kappa^{-1} \approx 9$ nm. Fitting formula (14) to the experimental data of Ref. 18 while imposing the constraint $B_{\rm co}(T_c) = 2B_0$, we extract the minimal length $l_{\rm min} \approx 1.2$ nm. Finally, formula (11) with $T_c \approx 60.7$ K determines the energy scale $\hbar v S \approx 0.12$ eV. Using $v \sim 2 \times 10^7$ cm s⁻¹ for the Fermi velocity, ²⁸ we find $S \sim 1$ nm⁻¹, i.e., the hot spots take several 10% of the Fermi surface.

These rough estimates fit our picture. In particular, the large ratio of the gapped Fermi surface supports the idea of hot spots coalescing and forming gapped regions that are centered at the antinodes and thus establish d-wave symmetry. ²⁹ At the same time, the estimates do not allow precise calculations of phase diagram parameters such as T^* or T_c since, in reality, the ratios between these scales are close to unity (T^* is just a few T_c). Nevertheless, the theoretical phase diagram in Fig. 1 illustrates well the experimental situation as reported in Ref. 18.

V. CONCLUSION

Studying in the presence of a magnetic field the microscopically derived theory of the pseudogap in high- T_c cuprates from Ref. 19, which is characterized by an SU(2) order parameter fluctuating between superconducting and charge order, we suggest an explanation for the unusual phase diagram including both orders and the pseudogap state observed experimentally in Ref. 18.

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