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Chiral symmetry breaking and phase fluctuations: A QED_3 theory of the pseudogap state in cuprate superconductors

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A *d*-wave superconductor, its phase coherence progressively destroyed by unbinding of vortex-antivortex pairs, suffers an instability related to chiral-symmetry breaking in QED_3. The chiral manifold exhibits large degeneracy spanned by physical states acting as inherent "competitors" of *d*-wave superconductivity. Two of these states are associated with antiferromagnetic insulator and "stripe" phases, known to be stable in the pseudogap regime of cuprates near half-filling. The theory also predicts an additional, yet unobserved state: a $d+ip$ phase-incoherent superconductor.

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Ever since the original discovery, the physics of high-temperature superconductors (HTS's) has been one of the key problems in theory of quantum condensed matter. The most actively pursued approach[1] is to focus on the insulating state of CuO_2 planes at half-filling and work one's way along the doping (x) axis to the *d*-wave superconductor. Alternatively, others have studied superconducting instabilities of a nearly antiferromagnetic Fermi liquid (FL).[2] Both approaches are examples of the traditional paradigm that "one should understand the normal state before one can understand the superconductor;" the strategy that has met with much success in conventional, low-T_c superconductors.

Recently, a different route toward the theory of HTS's has been advanced in Refs. 3 and 4. Cuprates are strongly interacting systems, where traditional approaches might be too forbidding. Instead, as argued in Ref. 4, one should focus on the superconducting state itself, which appears as the "least correlated" among its neighbors in the HTS phase diagram, and the integrity of its low-energy BCS-like quasiparticles protected by the large *d*-wave pseudogap. In this approach one considers the pseudogap regime as dominated by superconducting phase fluctuations and seeks to understand the "normal" states adjacent to a superconductor by focusing on the interaction between quasiparticles and vortex-antivortex excitations. There is considerable experimental evidence supporting this viewpoint.[5–9] In particular, recent Nernst effect measurements[7,9] indicate strong vortex fluctuations at temperatures comparable to the pseudogap ($T\sim T^*$) and far above the true T_c. The effective low-energy theory of these interactions was argued to be quantum electrodynamics in $(2+1)$ dimensions (QED_3).[4]

The success of this approach hinges on its ability, by using the *d*-wave superconducting state as its starting point, to reconstruct the general features of the HTS phase diagram. Amongst these, none is more prominent than the Néel antiferromagnetic insulator very near half filling. In this paper we first show that a *d*-wave superconductor whose phase coherence has been destroyed by the unbinding of quantum vortex-antivortex pairs indeed becomes an antiferromagnet.[10] The antiferromagnetism arises naturally through an inherent dynamical instability of QED_3, known as spontaneous chiral-symmetry breaking (CSB),[12] and most typically takes the form of an incommensurate spin-density wave (SDW), whose periodicity is tied to the Fermi surface. Furthermore, we next show that numerous other states, most notably a $d+ip$ and a $d+is$ *phase-incoherent* superconductor (dipSC, disSC) and "stripes," i.e., superpositions of one-dimensional charge-density waves (CDW) and *phase-incoherent* superconducting density waves (SCDW), as well as continuous chiral rotations among them, are all energetically close and competitive with antiferromagnetism due to their equal membership in the chiral manifold of two-flavor ($N=2$) QED_3. This large chiral manifold of nearly degenerate states plays the key role in our theory as the culprit behind the complexity of the HTS phase diagram.

The above results place tight restrictions on this phase diagram and provide means to unify the phenomenology of cuprates within a single, systematically calculable "QED_3 unified theory" (QUT). Any *microscopic* description of cuprates, as long as it leads to the large *d*-wave pairing pseudogap with $T^*\gg T_c\rightarrow 0$, will conform to the general results of QUT. In particular, all the physical states in natural energetic proximity to a *d*-wave superconductor are those inhabiting the above chiral manifold. Under the umbrella of the pseudogap, the energetics and various properties of such states are explicitly calculable from the chirally *symmetric* QED_3 theory of Ref. 4, which plays the role in the pseudogap state similar to that of the FL theory in conventional metals.

We now provide the substance behind the above assertions. Our starting point is the QED_3 Lagrangian

$$\mathcal{L}_{\mathrm{QED}}=\bar{\psi}_n c_{\mu,n}\gamma_\mu D_\mu \psi_n+\mathcal{L}_0[a_\mu]+(\cdots) \tag{1}$$

shown in Ref. 4 to desribe the low-energy effective theory for fermions in a *d*-wave superconductor interacting with dynamically fluctuating vortex excitations of the Cooper pair field. Here $\psi^\dagger_\alpha=\bar{\psi}_\alpha\gamma_0=(\eta^\dagger_\alpha,\eta^\dagger_{\bar{\alpha}})$ are the four-component Dirac spinors with $\eta^\dagger_\alpha=(1/\sqrt{2})\Psi^\dagger_\alpha(\mathbf{1}+i\sigma_1)$, $\eta^\dagger_{\bar{\alpha}}=(1/\sqrt{2})\Psi^\dagger_{\bar{\alpha}}\sigma_2(\mathbf{1}+i\sigma_1)$, and $\Psi^\dagger_\alpha=(\psi^\dagger_{\uparrow\alpha},\psi_{\downarrow\alpha})$. Fermion fields $\psi_{\sigma\alpha}(\mathbf{r},\tau)$ describe "topological fermions" of the theory and are related to the original nodal fermions

$c_{\sigma\alpha}(\mathbf{r},\tau)$ via the singular gauge transformation detailed in Refs. 4 and 13. Index n labels $(1,\bar{1})$ and $(2,\bar{2})$ *pairs* of nodes, while α labels individual nodes, $\mu=\tau,x,y$ $(\equiv 0,1,2)$. $D_\mu=\partial_\mu+ia_\mu$ is a covariant derivative, $c_{\tau,n}=1$, $c_{x,1}=c_{y,2}=v_F$, $c_{x,2}=c_{y,1}=v_\Delta$. The gamma matrices are defined as $\gamma_\mu=\sigma_3\otimes(\sigma_3,-\sigma_1,-\sigma_2)$ and satisfy $\{\gamma_\mu,\gamma_\nu\}=2\delta_{\mu\nu}$. The Berry gauge field a_μ encodes the topological frustration of nodal fermions generated by fluctuating quantum vortex-antivortex pairs and $\mathcal{L}_0$ is its bare Lagrangian. The loss of superconducting phase coherence caused by the unbinding of vortex pairs is heralded in Eq. (1) by a_μ becoming massless,[4]

$$\mathcal{L}_0\to\frac{1}{2e_\tau^2}(\partial\times a)_\tau^2+\sum_i\frac{1}{2e_i^2}(\partial\times a)_i^2; \tag{2}$$

here, $e_\tau^2, e_i^2 (i=x,y)$, as well as the velocities $v_{F(\Delta)}$, are functions of doping x and T. Along with residual interactions between nodal fermions, denoted by the ellipsis in Eq. (1), these parameters of QUT arise from some more microscopic description and will be discussed shortly.

First, however, we focus on the general properties of (1). The Berry gauge field a_μ is the main dynamical agent in our theory and plays a special role in the above expression. If we set $a_\mu=0$, all the remaining interactions among nodal fermions are short ranged, including those arising from the integration over the Doppler gauge field v_μ,[4] and irrelevant in the renormalization-group sense. They can impact the low-energy physics only through symmetry breaking and frequently first-order transitions. Consequently, if a_μ were absent or massive, such as in the superconducting state, the effective theory of the pseudogap state would be that of free, massless Dirac fermions. In contrast, a_μ is relevant in the massless (nonsuperconducting) state and it generates nontrivial long-range interactions among quasiparticles.[4] The effective theory of the pseudogap state is QED_3 and the low-energy physics is controlled by the *interacting* infrared fixed point of its *chiral-symmetric* (massless fermion) phase. This is the ''algebraic'' Fermi-liquid normal state discussed in Ref. 4.

$\mathcal{L}_{\mathrm{QED}}$ (1) possesses the following peculiar continuous symmetry: borrowing from ordinary quantum electrodynamics in $(3+1)$ dimensions (QED_4), we know that there exist two additional gamma matrices $\gamma_3=\sigma_1\otimes\mathbf{1}$ and $\gamma_5=i\sigma_2\otimes\mathbf{1}$ that anticommute with *all* γ_μ's. It is easy to show that $\mathcal{L}_{\mathrm{QED}}$ is invariant under $\psi_n\to e^{i\alpha\gamma_3}\psi_n$ and $\psi_n\to e^{\beta\gamma_5}\psi_n$, ($\alpha$, β real) defining a global U(2) symmetry for each pair of nodes with generators $\mathbf{1}\otimes\mathbf{1}$, γ_3, $-i\gamma_5$, and $\frac{1}{2}[\gamma_3,\gamma_5]$. In QED_3 this symmetry can be broken by two types of ''mass'' terms, $m_{\mathrm{ch}}\bar{\psi}_n\psi_n$ and $m_{\mathrm{PT}}\bar{\psi}_n\frac{1}{2}[\gamma_3,\gamma_5]\psi_n$. The phenomenon of spontaneous symmetry breaking in QED_3 as a mechanism for dynamical mass generation has been extensively studied in the quantum field theory literature.[12,14,15] Note that the chiral symmetry of our theory (1) is purely *dynamical*, i.e., it is not related to spin SU(2) or any other kinematic symmetry of the underlying microscopic Hamiltonian—we call it the Bogoliubov-deGennes (BdG) chiral symmetry. It has been established that while m_{PT} is never spontaneously generated,[14] the chiral mass m_{ch} is generated if the number of fermion species N is less than a critical value N_c. It is found that $N_c\sim 3$ for *isotropic* QED_3,[15,16] but as we shall discuss shortly, anisotropy and irrelevant couplings present in Lagrangian (1) can change the value of N_c. Furthermore, N itself, while equal to 2 for a single CuO_2 layer, could change to 4, 6, or an even larger value in bilayer and multilayer cuprates, thus enhancing the possibility of a symmetric $m_{\mathrm{ch}}=0$ phase.

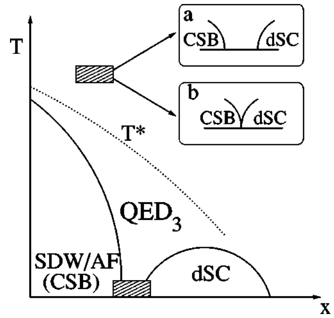

FIG. 1. Schematic phase diagram of a cuprate superconductor in QUT. Depending on the value of N_c (see text), either the superconductor is followed by a *symmetric* phase of QED_3, which then undergoes a quantum CSB transition at some lower doping [panel (a)], or there is a direct transition from the superconducting phase to the $m_{\mathrm{ch}}\neq 0$ phase of QED_3 [panel (b)]. The label SDW/AF indicates the dominance of the antiferromagnetic ground state as $x\to 0$.

Let us now assume that we are in the part of the phase diagram (Fig. 1) characterized by the parameters such that $N<N_c$: CSB occurs and the mass term $m_{\mathrm{ch}}\bar{\psi}_n\psi_n$ is generated. We wish to determine what is the nature of this chiral instability in terms of the original electron operators. To make this apparent, let us consider a general chiral rotation $\psi_n\to U_{\mathrm{ch}}^{(n)}\psi_n$ with $U_{\mathrm{ch}}^{(n)}=\exp(i\theta_{3n}\gamma_3+\theta_{5n}\gamma_5)$. Within our representation of Dirac spinors, Eq. (1), the $m_{\mathrm{ch}}\bar{\psi}_n\psi_n$ mass term takes the following form:

$$m_{\mathrm{ch}}\cos(2\Omega_n)[\eta_\alpha^\dagger\sigma_3\eta_\alpha-\eta_{\bar{\alpha}}^\dagger\sigma_3\eta_{\bar{\alpha}}] + m_{\mathrm{ch}}\sin(2\Omega_n)\frac{\theta_{5n}+i\theta_{3n}}{\Omega_n}\eta_\alpha^\dagger\sigma_3\eta_{\bar{\alpha}}+\mathrm{H.c.}, \tag{3}$$

where $\Omega_n=\sqrt{\theta_{3n}^2+\theta_{5n}^2}$. m_{ch} acts as an order parameter for the bilinear combinations of topological fermions appearing in Eq. (3). In the symmetric phase of QED_3 $(m_{\mathrm{ch}}=0)$, the expectation values of such bilinears vanish, while they become finite, $\langle\bar{\psi}_n\psi_n\rangle\neq 0$, in the broken-symmetry phase.

The BdG chiral manifold (3) is spanned by the ''basis'' of three symmetry-breaking states. When reexpressed in terms of the original nodal fermions $c_{\sigma\alpha}(\mathbf{r},\tau)$, two of these involve pairing in the particle-hole $(p\text{-}h)$ channel—a cosine and a sine spin-density wave (SDW),

$$\langle c_{\uparrow\alpha}^\dagger c_{\uparrow\bar{\alpha}}-c_{\downarrow\alpha}^\dagger c_{\downarrow\bar{\alpha}}\rangle+\mathrm{H.c.}\quad(\cos\mathrm{SDW}),$$

$$i\langle c_{\uparrow\alpha}^\dagger c_{\uparrow\bar{\alpha}}-c_{\uparrow\bar{\alpha}}^\dagger c_{\uparrow\alpha}\rangle+(\uparrow\to\downarrow)\quad(\sin\mathrm{SDW}), \tag{4}$$

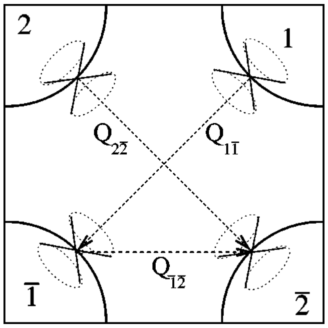

FIG. 2. The ''Fermi surface'' of cuprates, with the positions of nodes in the d-wave pseudogap. The wave vectors $\mathbf{Q}_{1\bar{1}}, \mathbf{Q}_{2\bar{2}}$, and $\mathbf{Q}_{\bar{1}2}$, etc. are discussed in the text.

and are obtained from Eq. (3) by setting Ω_n equal to $\pi/4$ or $3\pi/4$. Rotations within the BdG chiral manifold (3) at fixed Ω_n correspond to the sliding modes of SDW.

A simple physical picture emerges here: we started from a d-wave superconducting phase, our parent state. As one moves closer to half-filling and true phase coherence is lost, strong vortex-antivortex pair fluctuations, acting under the protective umbrella of a d-wave particle-particle (p-p) pseudogap, spontaneously induce formation of particle-hole ''pairs'' at finite wave vectors, $\pm\mathbf{Q}_{1\bar{1}}$ and $\pm\mathbf{Q}_{2\bar{2}}$, spanning the Fermi surface from node α to $\bar{\alpha}$ (Fig. 2). The glue that binds these p-h ''pairs'' and plays the role of ''phonons'' in this pairing analogy is provided by the Berry gauge field a_μ. Such ''fermion duality'' is a natural consequence of the QED_3 theory (1). Remarkably, we find the antiferromagnetic insulator being spontaneously generated in the form of the incommensurate SDW. As we get very near half-filling and $\mathbf{Q}_{1\bar{1}}, \mathbf{Q}_{2\bar{2}}$ approach $(\pm\pi,\pm\pi)$; SDW acquires the most favored state status within the BdG chiral manifold—this is the consequence of umklapp processes, which increase its condensation energy without it being offset by either the anisotropy or a poorly screened Coulomb interaction, which plagues its CDW competitors to be introduced shortly. It seems, therefore, reasonable to argue that this SDW must be considered the progenitor of the Neel-Mott-Hubbard insulating antiferromagnet at half-filling. Thus, QED_3 theory (1) explains the origin of antiferromagnetic order in terms of strong vortex-antivortex fluctuations in the parent d-wave superconductor. It does so naturally, through its inherent and well-established chiral-symmetry-breaking instability.[12]

The BdG chiral manifold (3) contains also a third state, a p-p pairing state corresponding to $\Omega_n = 0$ or $\pi/2$ and best characterized as a $d+ip$ phase-incoherent superconductor,

$$i\langle\psi_{\uparrow\alpha}\psi_{\downarrow\alpha}-\psi_{\uparrow\bar{\alpha}}\psi_{\downarrow\bar{\alpha}}\rangle+\text{H.c.}\quad (dip\text{SC}). \tag{5}$$

We have written dipSC in terms of topological fermions $\psi_{\sigma\alpha}(\mathbf{r},\tau)$, since the use of the original fermions leads to a more complicated expression, which involves the backflow of vortex-antivortex excitations. This state breaks parity but preserves time-reversal symmetry, translational invariance and superconducting U(1) symmetries. To our knowledge, such a state has not been proposed as a part of any of the major theories of HTS. It is an intriguing question whether this $d+ip$ phase-incoherent superconductor can be the actual ground state at some dopings in some of the cuprates. Its energetics does not suffer from long-range Coulomb problems but it is clearly inferior to the SDW very close to half-filling, since, being spatially uniform, it receives no help from the umklapp process. Observation of such a state in underdoped cuprates would provide strong evidence for the validity of the physical picture proposed in this paper.

Until now, we have discussed the CSB pattern only within individual pairs of nodes, $(1,\bar{1})$ and $(2,\bar{2})$, of a single CuO_2 plane. What happens if we allow for chiral rotations that mix nodes 1 and $\bar{2}$ or 1 and 2? A whole new plethora of states becomes possible, with the BdG chiral manifold enlarged to include a superposition of *one-dimensional* p-h and p-p states, an incommensurate CDW accompanied by a nonuniform phase-incoherent superconductor (SCDW) at wave vectors $\pm\mathbf{Q}_{12}$ and $\pm\mathbf{Q}_{\overline{21}}$ (Fig. 2):

$$\frac{1}{\sqrt{2}}\langle c^{\dagger}_{\uparrow 1}c_{\uparrow 2}+c^{\dagger}_{\uparrow\bar{2}}c_{\uparrow\bar{1}}+\text{H.c.}\rangle+(\uparrow\to\downarrow)\quad (\text{CDW}),$$

$$\frac{1}{\sqrt{2}}\langle\psi_{\uparrow 1}\psi_{\downarrow 2}+\psi_{\uparrow\bar{2}}\psi_{\downarrow\bar{1}}+\text{H.c.}\rangle+(\uparrow\leftrightarrow\downarrow)\quad (\text{SCDW}). \tag{6}$$

These same states, rotated by $\pi/2$, are replicated at wave vectors $\pm\mathbf{Q}_{1\bar{2}}$ and $\pm\mathbf{Q}_{2\bar{1}}$ (Fig. 2). In a fluctuating $d_{x^2-y^2}$ superconductor, these CDW's and SCDW's run along the x and y axes and are naturally identified as the ''stripes'' of QUT. Note, however, these are not the only one-dimensional states in QUT—among the states in the BdG chiral manifold (3) are also ''diagonal stripes,'' the combination of a SDW, Eq. (4), along $\pm\mathbf{Q}_{1\bar{1}}$ and a dipSC, Eq. (5), which opens the mass gap only at nodes $(2,\bar{2})$, or vice versa. Furthermore, a phase-incoherent $d+is$ superconductor (disSC) is also present within the chiral enlarged manifold, since it results in alternating signs for different nodes with equal number of positive and negative ''masses'' for the two-component nodal fermions:

$$i\langle\psi_{\uparrow 1}\psi_{\downarrow 1}+\psi_{\uparrow\bar{1}}\psi_{\downarrow\bar{1}}+\text{H.c.}\rangle+(1\to 2)\quad (dis\text{SC}). \tag{7}$$

In contrast, in a $d+id$ phase-incoherent superconductor these ''masses'' have the same sign for all the nodes producing a maximal breaking of the PT symmetry.[14] Consequently, a $d+id$ phase-incoherent superconductor is not spontanously induced within our QED_3 theory.

In the *isotropic* ($v_F = v_\Delta$) $N=2$ QED_3, all these additional states plus arbitrary *chiral* rotations among them are completely equivalent to those dicussed previously. It is here where we confront the problem of intrinsic anisotropy in Eq. (1). Such anisotropy cannot be rescaled out and manifestly breaks the $U(2)\times U(2)$ degeneracy of the full $N=2$ chiral manifold down to two separate $U(1)\times U(1)$ (3) chiral groups discussed previously. This is reflected in the general increase in energy of the states from the enlarged BdG chiral manifold. For example, the anisotropy raises the energy of our ''stripe'' states (6) relative to those of SDW, dipSC, or ''diagonal stripes.'' However, when the long-range Coulomb interactions and coupling to the lattice are included in the problem, as they are in real materials, it is conceivable that the "stripes" would return in some form, either as a ground state or a long-lived metastable state at some intermediate doping. disSC is also adversely affected by anisotropy but to a lesser extent and might remain competitive with SDW, dipSC, and "diagonal stripes."[17] This state breaks time-reversal symmetry but preserves parity and the discussion concerning dipSC below Eq. (5) applies to disSC equally well.

How do we use these general results on CSB in QUT to address the specifics of the cuprate phase diagram? To this end, we need some effective combination of phenomenology and more microscopic descriptions to determine the parameters v_F, v_Δ, e_τ, e_i and residual interactions $(\cdots)$ appearing in $\mathcal{L}_{\mathrm{QED}}$ (1). The main task is to determine what is the sequence of states within QUT that form stable phases as the doping decreases toward half-filling under T^* in Fig. 1. While this is an extensive project, whose detailed results will be reported elsewhere,[17] we outline here some of the general features. First, within the superconducting state $e_\tau, e_i \rightarrow 0$ and a_μ becomes massive, thus denying the CSB mechanism its main dynamical agent. We, therefore, expect that the superconductor is in the symmetric phase and its nodal fermions form well-defined excitations.[4] As we move to the left in Fig. 1, the phase order is suppressed and e_τ, e_i become finite, reflecting the unbinding of vortex-antivortex excitations.[4] For all practical purposes, this is precisely what the experiments imply. Now, the key question is whether the QED_3 (1) remains in its symmetric phase or whether it immediately undergoes the CSB transition and generates finite gap ($m_{\mathrm{ch}} \neq 0$).

One important factor in the above problem is the dependence of N_c on the Dirac cone anisotropy $\alpha_D = v_F/v_\Delta$. This is a technically nontrivial problem, which we shall discuss elsewhere.[17] Our preliminary results suggest that N_c is a weakly increasing function of α_D (see also Ref. 11). In the superconducting state the anisotropy is fairly large, $\alpha_D \simeq 10 - 20$.[18] This would then favor a direct transition into the broken-symmetry phase [panel (b) of Fig. 1], which could conceivably become first order with a region of coexisting antiferromagnetic order and superconductivity. If, on the other hand, $N_c < \frac{3}{2}$ as argued in Ref. 16, there could be a locus of doping concentration in which ground state is nonsuperconducting but chirally symmetric [panel (a) of Fig. 1]. Such an intermediate symmetric phase is particularly likely in bilayer or multilayer cuprates (such as YBCO or $\mathrm{HgBa_2Ca_2Cu_3O_8}$), where highly anisotropic interlayer hopping translates into strong coupling between vortices but essentially no coupling between nodal fermions on constituent $\mathrm{CuO_2}$ planes, thus raising the N of QED_3 (1) to 4, 6, or even higher, and above N_c.

The anisotropy is not the only factor that can influence the value of N_c. Short-range interactions, while perturbatively irrelevant, effectively increase N_c if stronger than some critical value.[19] Such interactions, typically in the form of short-range three-current terms,[3] arise in more microscopic models used to derive $\mathcal{L}_{\mathrm{QED}}$ (Ref. 17) and are prominent among the residual terms denoted by the ellipsis in Eq. (1). Their strength generically increases as $x \rightarrow 0$. These residual interactions play a dual role in QUT. First, they can conspire with the anisotropy to produce the situation depicted in panel (b) of Fig. 1, where the CSB takes place as soon as the phase coherence is lost. Second, once the chiral symmetry has been broken, the residual interactions further break the symmetry within the chiral manifold (3) and play a role in selecting the true ground state. A detailed analysis of the CSB patterns will be reported separately.[17]

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