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Magnetic field induced charge and spin instabilities in cuprate superconductors

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A d -wave superconductor, subject to strong phase fluctuations, is known to suffer an antiferromagnetic instability closely related to the chiral symmetry breaking in (2+1)-dimensional quantum electrodynamics (QED₃). Based on this idea we formulate a “QED₃ in a box” theory of *local* instabilities of a d -wave superconductor in the vicinity of a single pinned vortex undergoing quantum fluctuations. As a generic outcome we find an incommensurate 2D spin density wave forming in the neighborhood of a vortex with a concomitant “checkerboard” pattern in the local electronic density of states, in agreement with recent neutron scattering and tunneling spectroscopy measurements.

Among the open questions in modern condensed matter physics, few have inspired more theoretical effort than the emergence of a superconducting state from the doped antiferromagnetic (AF) insulator [1]. Recently, using an “inverted” approach to the problem [2, 3], it has been shown that AF order arises naturally when the superconducting order in a d -wave superconductor (d SC) is destroyed by vortex-antivortex fluctuations [4, 5]. As we shall discuss, the implications of these theories transcend the possibility of providing a route to understanding the destruction of superconductivity in strongly-underdoped cuprates; indeed, they also apply to the problem of *local* field-induced vortices within the superconducting state.

Recent neutron scattering [6, 7] and scanning tunneling spectroscopy (STS) [8] experiments have revealed the presence of local AF and charge order in the vicinity of field-induced vortices. Existing theoretical treatments [9, 10, 11, 12, 13] of vortex-induced AF ordering rely on the proximity of the system to a quantum critical point. Within such treatments, it is the suppression of the SC order parameter near the vortex cores that leads to the nucleation of islands of AF order. Here we present an alternative scenario in which the AF order is brought about by *local quantum fluctuations* of a vortex around its equilibrium position. In the present theory there is no competition between the SC amplitude and AF order: the latter arises purely from the presence of vortex fluctuations and is a genuine low-energy phenomenon taking place on lengthscales much longer than the core size.

It is a well-known fact that the low superfluid density in cuprates makes the SC order vulnerable to phase fluctuations [14, 15, 16]. This observation has inspired theories in which the pseudogap state is modeled as a phase-disordered d -wave superconductor [2, 3, 17, 18], such that the demise of superconductivity is brought about by the unbinding and proliferation of the topological defects – vortices – in the phase of the SC order parameter. It has been pointed out [3] that fluctuating vortices produce a non-trivial Berry-phase interaction between the quasiparticles of the underlying d SC. This interaction is described in terms of a massless non-compact gauge field a_μ , minimally coupled to the Dirac fermions representing the low-energy quasiparticle excitations of the system. Within the theory of Ref. [3] which

maps the problem onto (2+1)-dimensional quantum electrodynamics (QED₃), it is this interaction that destroys the Fermi liquid nature of quasiparticles in the pseudogap state and ultimately drives the AF instability [4, 5]. Remarkably, both the ‘algebraic’ Fermi liquid describing the symmetric pseudogap phase and the antiferromagnet emerge from the same QED₃ theory [3].

Here, we use the philosophy and formalism developed in Refs. [3, 4, 5] to model quasiparticle excitations in the *superconducting state* in the spatial region close to a single field-induced vortex undergoing fluctuations around its equilibrium position. We call this model “QED₃ in a box”. We note that there exists direct experimental evidence that individual vortices indeed undergo significant quantum fluctuations [19]. We find that, under generic conditions, interactions generated by such fluctuating vortex lead to *local* instability of the superconducting state which takes form of a 2D incommensurate AF spin density wave (SDW) with a wave vector tied to the positions of the nodes in the underlying d -wave gap.

In order to motivate our model for a single vortex we first review the treatment of the AF instability in QED₃ and reformulate it in a way that will be more suitable for our present purposes. We start from the Euclidean QED₃ action $S = \int d^3x \mathcal{L}_D$ with

$$\mathcal{L}_D \equiv \sum_{l=1}^N \bar{\Psi}_l(x) \gamma_\mu (i\partial_\mu - a_\mu) \Psi_l(x) + \mathcal{L}_B[a(x)], \quad (1)$$

describing the low-energy fermionic excitations of a d -wave SC coupled to fluctuating vortices represented by the gauge field a_μ [3]. Here, $\Psi_l(x)$ is a four component Dirac spinor representing the fermionic excitations associated with a pair of antipodal nodes, $x = (\tau, \mathbf{r})$ denotes the space-time coordinate, and γ_μ ($\mu = 0, 1, 2$) are the gamma matrices satisfying $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$. The number N of fermion species is equal to 2 for single-layer cuprates; $N = 4, 6, \dots$ for bilayer, trilayer and multilayer materials. The Lagrangian \mathcal{L}_B encodes the dynamics of the gauge field a_μ and is given by $\mathcal{L}_B[a] = \Pi_{\mu\nu}(q) a_\mu(q) a_\nu(-q)$ with

$$\Pi_{\mu\nu}(q) = \left(m_a + \frac{N}{8} |q| \right) \left(\delta_{\mu\nu} - \frac{q_\mu q_\nu}{q^2} \right). \quad (2)$$

The gauge field mass m_a vanishes when vortices are unbound (i.e., in the pseudogap regime or, in the present situation, near a single fluctuating vortex) and is finite in the superconducting state where vortices appear only in tightly bound loops or pairs.

In the standard treatment [4, 5] the AF order occurs via the phenomenon of chiral symmetry breaking [20, 21, 22] in the QED₃ Lagrangian (1). The instability is signaled by the spontaneous generation of fermion mass, m_D , which is interpreted in our context as the onset of SDW gap [4, 5] for the original Bogoliubov quasiparticles. The most general, nonperturbative treatment of mass-generation in QED₃ obtains m_D as a solution of a self-consistent Dyson-Schwinger equation. Here we shall follow a slightly simpler route which leads to the same result and has the advantage of being more easily generalizable to the present problem. In Eq. (1) we integrate out the gauge field to obtain the following fermionic effective action:

$$S_{\text{eff}} = \int d^3x \bar{\Psi}(x) \gamma_\mu i \partial_\mu \Psi(x) - \int d^3x \int d^3y J_\mu(x) D_{\mu\nu}(x-y) J_\nu(y), \quad (3)$$

where $J_\mu(x) \equiv \bar{\Psi}(x) \gamma_\mu \Psi(x)$ is the fermion 3-current and $D_{\mu\nu}(x)$ is the Fourier transform of the gauge boson propagator $D_{\mu\nu}(q) = \Pi_{\mu\nu}^{-1}(q)$. Henceforth we shall focus on a single pair of nodes and thus drop the nodal index l . The integrand of the interaction term may be written as $D_{\mu\nu}(x-y) \text{Tr}[\Psi(y) \bar{\Psi}(x) \gamma_\mu \Psi(x) \bar{\Psi}(y) \gamma_\nu]$ where the trace is taken over the spinor indices. This form suggests a Hartree-Fock (HF) approach in which we decouple the 4-fermion interaction to obtain $D_{\mu\nu}(x-y) \text{Tr}[\Psi(y) \bar{\Psi}(x) \gamma_\mu G_0(x, y) \gamma_\nu]$ with $G_0(x, y) = \langle \Psi(x) \bar{\Psi}(y) \rangle$ and the average is taken with respect to the HF effective action to be specified shortly. To make the structure of the interaction term more transparent we utilize the relative and center of mass coordinates $r = x - y$ and $R = (x + y)/2$ to write it as

$$\int d^3R \int d^3r \text{Tr} [\Psi(R_+) \bar{\Psi}(R_-) \gamma_\mu G_0(R, r) \gamma_\nu] D_{\mu\nu}(r), \quad (4)$$

where $R_\pm \equiv R \pm \frac{r}{2}$. In the *uniform* system the Green's function is independent of R , $G_0(R, r) = G_0(r)$. Furthermore, both $G_0(r)$ and $D_{\mu\nu}(r)$ are strongly peaked at $r \rightarrow 0$. The dominant contribution to the interaction therefore comes from this region and we may write (4) as [23]

$$\int d^3R \bar{\Psi}(R) \Psi(R) \int d^3r \gamma_\mu G_0(r) \gamma_\nu D_{\mu\nu}(r). \quad (5)$$

We have dropped the trace since the interaction is proportional to the unit matrix in the spinor space.

Inspection of Eq. (5) suggests the following HF effective

action and self-consistency condition:

$$S_{\text{HF}} = \int d^3x \bar{\Psi}(x) (\gamma_\mu i \partial_\mu - i m_D) \Psi(x), \quad (6a)$$

$$i m_D = \frac{1}{4} \text{Tr} \int d^3r \gamma_\mu G_0(r) \gamma_\nu D_{\mu\nu}(r). \quad (6b)$$

The last integral is easily evaluated by going to momentum space and Eq. (6b) becomes $m_D = (8m_D/N\pi^2) \ln(\Lambda/m_D)$, where Λ is the high-momentum cutoff. This yields a nontrivial solution

$$m_D = \Lambda e^{-N\pi^2/8}, \quad (7)$$

in agreement with the classic result of Pisarski [20]. More sophisticated treatments [21, 22] based on the Schwinger-Dyson equation give a finite critical value of N_c above which no mass is generated; however, for our purposes the level of approximation embodied by Eq. (7) will be sufficient.

We have thus seen that, in a uniform system, fluctuating vortices lead to the formation of SDW order. The challenge we now face is twofold: (i) we must adapt the above treatment to the case of a single fluctuating vortex, and (ii) since we seek to study the commensuration effects present in real materials, we must formulate the corresponding theory on the lattice. To address (i) let us denote by ℓ_v the characteristic length scale over which the vortex fluctuates around its classical equilibrium position. Within this length scale, the Berry-phase interaction between quasiparticles (and hence tendency towards SDW ordering) will be strong. We model this by taking in this region the gauge field to be *massless*. On the other hand at distances well beyond ℓ_v , quasiparticles feel no interaction and we model this by gauge field having a large mass m_a . In particular we take,

$$m_a(\mathbf{R}) = \Delta_0 \left(\frac{|\mathbf{R}|}{\ell_v} \right)^n, \quad (8)$$

where Δ_0 is an energy scale which we take to be the maximum superconducting gap, $|\mathbf{R}|$ is the distance from the vortex equilibrium position and n is a positive exponent. (We use $n = 2$ but our numerical calculations below are largely insensitive to the exact value of n .)

To address (ii), (i.e., to put the theory on the lattice) we recall that the effective action (1) and its HF version Eq. (6a) descend from a model of a lattice d SC linearized near the nodes of the gap. We therefore consider the corresponding lattice Hamiltonian enriched by the ‘‘mass’’ term present in Eq. (6a), to represent the HF decoupled Berry phase interaction. Thus we have,

$$H_{\text{HF}} = \sum_\sigma \sum_{\langle ij \rangle} \Phi_{i\sigma}^\dagger \mathcal{H}_{ij}^\sigma \Phi_{j\sigma}. \quad (9)$$

Here $\Phi_{i\sigma}^\dagger = (c_{i\sigma}^\dagger, c_{i\bar{\sigma}}^\dagger)$, $c_{i\sigma}^\dagger$ represents the electron creation operator at lattice site i , spin index $\bar{\sigma} = -\sigma$, and

$$\mathcal{H}_{ij}^\sigma = \begin{pmatrix} -t_{ij} + \delta_{ij}(m_{i\sigma} - \mu) & \Delta_{ij} \\ \Delta_{ij}^* & t_{ij} - \delta_{ij}(m_{i\bar{\sigma}} - \mu) \end{pmatrix},$$

with t_{ij} the tight binding hopping amplitude, Δ_{ij} the SC gap, μ chemical potential, and $m_{i\sigma}$ the local spin magnetization representing the mass gap m_D in Eq. (6a).

We diagonalize H_{HF} by the generalized Bogoliubov transformation $c_{i\sigma} = \sum_n [u_{n\sigma}(\mathbf{r}_i)\gamma_{n\sigma} + \sigma v_{n\bar{\sigma}}^*(\mathbf{r}_i)\gamma_{n\bar{\sigma}}^\dagger]$, where $\chi_{n\sigma}(\mathbf{r}_i) \equiv [u_{n\sigma}(\mathbf{r}_i), \sigma v_{n\sigma}(\mathbf{r}_i)]^T$ satisfy

$$\sum_j \mathcal{H}_{ij}^\sigma \chi_{n\sigma}(\mathbf{r}_j) = \epsilon_{n\sigma} \chi_{n\sigma}(\mathbf{r}_i). \quad (10)$$

In terms of the $\chi_{n\sigma}$, the self-consistency condition (6b) can be written as

$$m_{i\sigma} = \sum_{n\sigma j} \sigma f(\epsilon_{n\sigma}) V_i(\mathbf{r}_j) u_{n\sigma}^*(\mathbf{R}_i + \mathbf{r}_j) u_{n\sigma}(\mathbf{R}_i - \mathbf{r}_j),$$

$$V_i(\mathbf{r}) \equiv \frac{1}{4} \int_0^\infty d\tau e^{-\tau \epsilon_{n\sigma}} \text{Tr} [\gamma_\mu D_{\mu\nu}(\tau, \mathbf{r}) \gamma_\nu]. \quad (11)$$

For $m_a \neq 0$ the above integral cannot be evaluated in closed form. However, we find that it can be accurately approximated by a simple interpolation formula

$$V_i(\mathbf{r}) \simeq \mathcal{V}_0 \frac{c_1}{r(r m_a(\mathbf{R}_i) + c_1)(r \epsilon_{n\sigma} + c_1)} \quad (12)$$

where $r = |\mathbf{r}|$, $c_1 = 2/\pi$ and $\mathcal{V}_0 = 16/N\pi^2$ for the case of an isotropic Dirac cone ($t = \Delta$). In the physical case $t > \Delta$ the constant \mathcal{V}_0 will be modified somewhat and in what follows we treat it as an adjustable parameter of the model measuring the strength of the interaction. It is interesting to note that, as seen from Eq. (12), in (2+1)D a gauge field mass does *not* lead to exponentially decaying interactions on long length scales.

To capture the effect of vortex fluctuations on the local superconducting order we solve the eigenproblem (10) numerically on a lattice of $M \times M$ sites and iterate to self-consistency using Eq. (11). For simplicity we consider only nearest-neighbor hopping amplitudes $t_{ij} = t$ and a uniform d -wave gap $\Delta_{ij} = \pm \Delta_0$, with + and - signs referring to vertical and horizontal bonds respectively. We emphasize that the vortex, fluctuating around the equilibrium position at the center of our lattice, enters through the position dependent gauge-field mass $m_a(\mathbf{R})$ given by Eq. (8), which in turn enters the potential $V_i(\mathbf{r})$ given by Eq. (12). In the spirit of our working philosophy that the SDW order arises from the vortex fluctuations (and therefore from the gauge field), we neglect at this stage any effects of the superflow around the vortex or suppression of Δ_{ij} in the core. Such effects are well understood and will be included in a future publication. We also neglect the effects of changes in the fermionic spectrum due to the onset of SDW on the interaction mediated by Berry gauge field Eq. (12).

The diagonalizations are performed using standard LAPACK routines, which allow us to handle systems up to 40×40 sites. Typically, 10-15 iterations are needed to ensure self-consistency in $m_{i\sigma}$. We use both periodic and free boundary conditions and find that they have negligible effect on the results reported below. Our typical results are summarized in Figs. 1 and

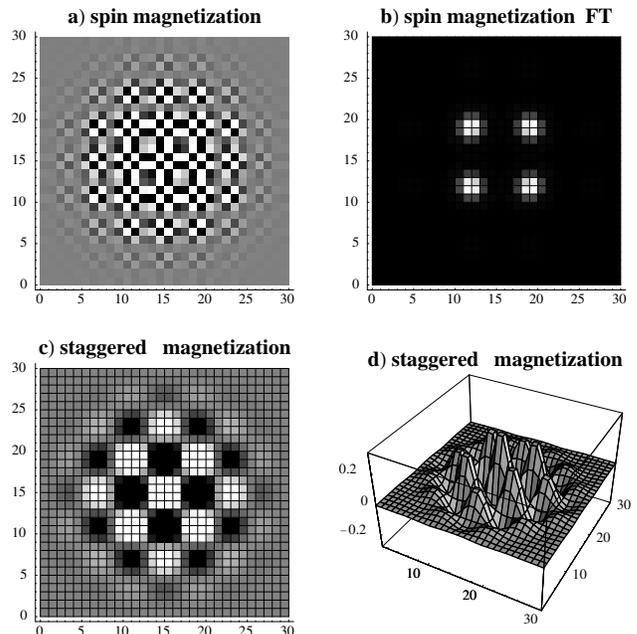


FIG. 1: Magnetization M_i and staggered magnetization M_i^S induced in the vicinity of the fluctuating vortex. Parameters used: $t = 1$, $\Delta_0 = 0.7$, $\mu = -1.6$ resulting in maximum gap of 2.3 and average charge density $n = 0.62$ electrons per site, $\mathcal{V}_0 = 1.0$ and $\ell_v = 12$; periodic boundary conditions.

2, showing the spatial distributions of the spin magnetization $M_i = \sum_\sigma \sigma \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle$, staggered spin magnetization $M_i^S = M_i (-1)^{x_i + y_i}$, local electron charge density $n_i = \sum_\sigma \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle$, and energy integrated local density of states (LDOS) $S_{E_1}^{E_2}(i) = \int_{E_1}^{E_2} \rho_i(E) dE$ where $\rho_i(E)$ is the LDOS at site i , as well as their respective Fourier transforms (FTs).

Panel (a) in Fig. 1 illustrates the “2D” incommensurate SDW pattern emerging in the vicinity of a fluctuating vortex with an 8×8 unit cell containing islands of AF order separated by anti-phase domain walls [apparent in panel (c)]. The FT displayed in panel (b) reveals that this pattern can be thought of as a superposition of four 1D SDWs with wave vectors $\mathbf{Q}_{\text{SDW}} = \pi(1 \pm \delta_{\text{SDW}}, 1 \pm \delta_{\text{SDW}})$, $\delta_{\text{SDW}} = \frac{1}{4}$. The size of δ_{SDW} is doping dependent: it shrinks with increasing μ and vanishes at half filling ($\mu = 1$), giving rise to perfectly commensurate AF SDW. We also find that for $\mu < -1.7$ the SDW becomes very weak for reasonable values of coupling \mathcal{V}_0 : overdoped samples are less susceptible to AF instability.

According to general symmetry arguments, a spatial modulation in the spin density generates a modulation in the charge density, $\delta n_i \propto M_i^2$. For our 2D SDW pattern this implies that the corresponding CDW will have a unit cell with half the area, rotated by 45° relative to the unit cell of M_i^S . Indeed, panels (a) and (b) of Fig. 2 confirm this general expectation, showing a “checkerboard” CDW at principal wavevectors $\mathbf{Q}_{\text{CDW}} =$

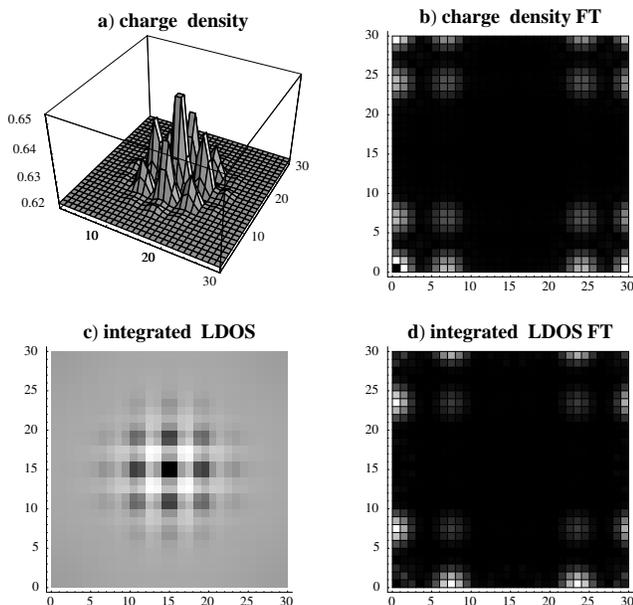


FIG. 2: Local charge density n_i and integrated LDOS $S_{0.2}^{0.7}(i)$ for the same parameters as Fig. 1.

$\pi(\pm\delta_{\text{CDW}}, 0), \pi(0, \pm\delta_{\text{CDW}})$ with $\delta_{\text{CDW}} = \frac{1}{2}$. A similar checkerboard pattern arises in the integrated LDOS and is displayed in panels (c) and (d).

Our findings of a checkerboard pattern in LDOS are consistent with the recent STS experiments performed on $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (BSCCO) crystals [8]. Our prediction is that the period of the pattern should increase with underdoping and that the effect should vanish in the overdoped samples. Also, if the observed LDOS pattern is associated with electron density modulation in a single CuO layer, we predict that the corresponding neutron scattering peaks should be found at wavevectors

$\mathbf{Q}_{\text{SDW}} = \pi(1 \pm \frac{1}{4}, 1 \pm \frac{1}{4})$. We note that neutron experiments [6, 7] on $\text{La}_{1.84}\text{Sr}_{0.16}\text{CuO}_4$ (LSCO) show peaks at different k -space positions, $\pi(1 \pm \frac{1}{4}, 1)$ and $\pi(1, 1 \pm \frac{1}{4})$. Although the findings of STS and neutron experiments are generally cited as being mutually consistent our analysis above indicates that this is not necessarily so: for a genuine 2D SDW illustrated in Fig. 1 determination of the corresponding CDW must consider the interference terms which cause the apparent 45° rotation of the latter. In the absence of neutron measurements on BSCCO we see two possible resolutions of this difficulty. First, it may be that the CDW pattern is truly 2D and neutron scattering on BSCCO would find a pattern illustrated in Fig. 1(b). Second, it could be that STS sees an incoherent superposition of two orthogonal 1D CDWs originating in two CuO layers comprising the BSCCO bilayer. This would explain the $x - y$ anisotropy reported in Ref. [8] and the neutron pattern would be consistent with that observed in LSCO. Within our simple model such 1D solutions have slightly higher energy than the 2D solutions reported above but it is possible that in a more complete model (using e.g. a more realistic band structure) the situation will be reversed.

To summarize, we have presented a “QED₃ in a box” theory for field induced spin and charge instabilities in cuprates, driven by local fluctuations of a pinned vortex. Without any need to fine-tune parameters we find LDOS patterns in detailed agreement with the tunneling data on BSCCO [8] and we relate them in a plausible way to existing neutron experiments [6, 7]. Other models [9, 10, 11, 12, 13] rely on the local suppression of the superconducting order parameter and would therefore predict similar instabilities in the vicinity of impurities, grain boundaries, and sample edges where thus far no such effects have been observed.

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