MAGNETIC FIELD TUNING OF CHARGE AND SPIN ORDER IN THE CUPRATE SUPERCONDUCTORS

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Recent neutron scattering, nuclear magnetic resonance, and scanning tunneling microscopy experiments have yielded valuable new information on the interplay between charge and spin density wave order and superconductivity in the cuprate superconductors, by using an applied perpendicular magnetic field to tune the ground state properties. We compare the results of these experiments with the predictions of a theory which assumed that the ordinary superconductor was proximate to a quantum transition to a superconductor with co-existing spin/charge density wave order.

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1 Introduction

An innovative series of recent experiments [1-4] have shed new light on the nature of strong correlations in the cuprate superconductors. These experiments all use a magnetic field, applied perpendicular to the CuO_2 layers, to tune the low temperature properties of the superconducting state. Their results support the idea that ground state correlations in the doped Mott insulator can be described using a framework of competing order parameters [5-8]. In our view, they (especially [4]) also offer compelling evidence that the orders competing with the superconductivity are spin and charge density waves, and suggest that one or both are present in the insulating state at very high fields [9].

In the underdoped regime, experimental evidence for spin and charge density ordering, coexisting with superconductivity, has accumulated over the last decade [5,10-13]. With increasing doping, some experimental results [13,14] can also be explained by proximity to a quantum critical point at which the spin/charge order disappears. At optimal doping, it is widely accepted that the important qualitative characteristics of the ground state are identical to those of a d-wave superconductor described in the standard BCS-BdG theory; nevertheless even at such dopings an attractive description of the collective spin and charge excitations is provided by a theory of the vicinity of the spin/charge ordering critical point at lower doping [15]. Such a framework was used recently [16,17] to address the influence of the applied magnetic field, and a number of its specific predictions appear to have been confirmed in subsequent measurements [2-4]. Here we will briefly review aspects of this theory and discuss extensions needed to develop a complete theory of the remarkable recent scanning tunneling microscopy (STM) measurements of Hoffman *et al.* [4].

2 Order parameters and quantum field theory

We consider a zero temperature transition between a d-wave superconductor (SC) and a superconductor with co-existing spin/charge order (SC+SDW/CDW). The density wave order parameters for the transition are defined by the following representations of spin ($S_\alpha(\mathbf{r},\tau)$, $\alpha = x, y, z$) and charge density modulation ($\delta\rho(\mathbf{r},\tau)$) at imaginary time τ and on the sites, $\mathbf{r}$, of a square lattice with unit lattice spacing:

$$S_\alpha(\mathbf{r},\tau) = \mathrm{Re}\left(\Phi_\alpha(\mathbf{r},\tau)\, e^{i\mathbf{K}_s\cdot\mathbf{r}}\right) \quad ; \quad \delta\rho(\mathbf{r},\tau) = \mathrm{Re}\left(\phi(\mathbf{r},\tau)\, e^{i\mathbf{K}_c\cdot\mathbf{r}}\right), \tag{1}$$

where $\mathbf{K}_s$ and $\mathbf{K}_c$ are the respective ordering wavevectors. A phase with SDW order has $\langle\Phi_\alpha\rangle \neq 0$ and a broken spin rotation symmetry; it is important to note that we use the term 'CDW order' (with $\langle\phi\rangle \neq 0$) in its most general sense: all local observables which are invariant under spin-rotation and time-reversal symmetries (like the on-site energy, or the bond kinetic and exchange energies, or the bond charge density) acquire a spontaneous modulation at wavevector $\mathbf{K}_c$, and it is possible that the modulation in the total site charge density itself is quite small. Excluding the case of two sublattice orderings (with wavevectors $(\pi,\pi), (\pi,0), (0,\pi)$), the order parameters Φ_α, ϕ are *complex fields*, with their phases representing a sliding degree of freedom of the density wave. This sliding degree of freedom is also present when the ordering is commensurate, but the phases then prefer to take a discrete set of values. We will focus here on the case $\mathbf{K}_s = (3\pi/4, \pi)$, $\mathbf{K}_c = (\pi/2, 0)$ which is experimentally relevant above a doping of about 1/8 (a theoretical rationale for the selection of this value of $\mathbf{K}_c$ was provided in [18]); the generalization to other commensurate and incommensurate wavevectors is immediate. The theory also includes order parameters associated with density waves in the orthogonal direction ($\mathbf{K}_s' = (\pi, 3\pi/4)$, $\mathbf{K}_c' = (0, \pi/2)$) but we will not write down these terms explicitly in the interest of brevity—this has been done in [17]. A variety of SDW and CDW phases (with background SC order) are possible in models described by the fields Φ_α and ϕ, and some of these have been described in [19]. Here we will focus on the simplest possibility of a transition from SC to SC+SDW driven by the condensation of Φ_α (results are similar in other cases); as discussed in [19] the condensation of Φ_α also leads to concomitant CDW order with $\mathbf{K}_c = 2\mathbf{K}_s$ (modulo a reciprocal lattice vector), and near the transition we can pin the charge order field to the spin order field by

$$\phi(\mathbf{r},\tau) \propto \Phi_\alpha^2(\mathbf{r},\tau) \tag{2}$$

where a summation over the repeated index α is implied here and henceforth.

The effective action for Φ_α describing the quantum transition from SC to SC+SDW is [6,7,15-19]:

$$S_\Phi = \int d^2\mathbf{r}\, d\tau \; \left[|\partial_\tau \Phi_\alpha|^2 + c_x^2 |\partial_x \Phi_\alpha|^2 + c_y^2 |\partial_y \Phi_\alpha|^2 + s\, |\Phi_\alpha|^2 + \frac{u_1}{2}\left(|\Phi_\alpha|^2\right)^2 \right.$$

$$+\frac{u_2}{2}\left|\Phi_\alpha^2\right|^2+\lambda\left(\left(\Phi_\alpha^2\right)^4+\text{c.c.}\right)\Bigg] \tag{3}$$

where $c_{x,y}$ are velocities, and s is a coupling which tunes the system across the SC to SC+SDW transition. We have neglected couplings to the fermionic nodal quasiparticles as we assume they have been suppressed by constraints from momentum conservation [16,17]. The non-linearity u_2 selects between spiral and collinear spin orderings [19,17], and we assume $u_2 < 0$, for which case collinear ordering with $\epsilon_{\alpha\beta\gamma}\langle\Phi_\beta\rangle\langle\Phi_\gamma^*\rangle = 0$ is selected, as is the case experimentally. The λ term is special to the value $\mathbf{K}_s = (\pi/4, 0)$ and prefers that the phase of Φ_α take a set of discrete values: it is permitted for this value of $\mathbf{K}_s$ because translations by integer lattice spacings correspond to the discrete transformation (see (1))

$$\Phi_\alpha \to \Phi_\alpha e^{in\pi/4},\ n \text{ integer}, \tag{4}$$

under which all the terms in S_Φ are invariant; the sign of λ chooses between bond and site centered density waves [17].

The SC phase with no SDW order is realized for s larger than some critical value s_c. An important property of this phase is that the Φ_α quanta constitute a stable excitonic excitation with a *6-fold* degeneracy. At the Gaussian level this is evident from the fact that the quadratic terms in (3) have a global O(6) symmetry. However, the terms proportional to u_2 and λ are only invariant under O(3) spin rotation symmetry and the discrete symmetry (4), but a perturbative computation to all orders easily shows that this symmetry is sufficient to preserve the 6-fold degeneracy. The usual degeneracy of a spin $S = 1$ triplet has been doubled by the additional discrete sliding degree of freedom of the SDW.

Now let us consider the influence of an applied magnetic field, H, on the SC phase. An important early contribution was made by Arovas *et al.* [20] who focused on cores of the vortices in the SC order introduced by H and argued that, because of a microscopic repulsion between the SC and Néel orders, locally the SC order would "rotate" into an insulating Néel (SDW) phase. The cores have since been examined in a number of experiments [21,22,3] and no clear sign of such behavior emerged: instead the sub-gap conductance is enhanced in the cores, additional core states appear, and there may be a subdominant pairing amplitude (*e.g.* $d_{x^2-y^2} + id_{xy}$) [23]. The nuclear magnetic resonance (NMR) experiments observed enhanced antiferromagnetic *fluctuations* located *outside* the vortex core, as was originally predicted in [16] (see below); the formalism of [20] allows static antiferromagnetic order on scales larger than the core size, and this along with the extension to dynamic antiferromagnetism was discussed recently in [24].

Two of us and Y. Zhang [16] examined the consequences of the microscopic repulsion between SC and SDW orders, but near a bulk transition between the SC and SC+SDW phases. We argued that effects driven by the strongly relevant $u_{1,2}$ interactions in (3) implied that the predominant enhancement of the SDW fluctuations in the SC phase, and the consequent lowering of the exciton energy, occurred primarily in the superconducting region outside the vortex cores, driven by the superflow induced by H. (Loosely speaking, this can be understood as follows: as we approach the onset of SDW order by decreasing s, Φ_α initially attempts to condense in the cores of the vortices. However, the quartic self interactions $u_{1,2}$

are most effective in this strongly localized region, and this drives up the effective Hartree potential felt by Φ_α in the core. So Φ_α can only condense in an extended state which is primarily sensitive to the large spatial region outside the core over which the superflow is present. Alternatively stated, the energy of any Φ_α states which may be localized in the core *always* remains at non-zero energies of order of the exchange interaction (and so are probably strongly overdamped), and Bose condensation of Φ_α can only occur in extended states outside the core whose energy can indeed approach zero [25].) These predictions appear to have been confirmed in subsequent experiments: the NMR experiments of [3] were noted above, and the recent STM measurements of [4] observe CDW modulations (which are related to the SDW by (2)) at distances almost an order of magnitude beyond the point where the superconducting coherence peaks are fully recovered outside the vortex core. The work of [16] also made predictions on the H-dependence of the elastic Bragg peaks associated in the SC+SDW phase: these are in good accord with subsequent neutron scattering measurements [2].

We briefly mention the field theory origin of the results of [16]. As we are focusing on long length scales outside the small vortex cores, a continuum description is possible. For the collective spin/charge excitations we use S_Φ in (3); for simplicity, we do not include a Zeeman coupling to H in S_Φ because it only modifies physical properties at order H^2 (because, loosely speaking, the average field on the spins in the oscillating SDW vanishes). The infinite diamagnetic susceptibility of the SC order makes its response to H much stronger, and we describe this, and the coupling to Φ_α, by the action $S_\Phi + S_\Psi$ (this cannot be applied within the core where the SC wavefunction is perturbed in different ways, as noted above), where

$$S_\Psi = \int d^2 r d\tau \left[\left|(\nabla - i\mathbf{A})\,\Psi\right|^2 - |\Psi|^2 + \frac{|\Psi|^4}{2} + \kappa\,|\Psi|^2\,|\Phi_\alpha|^2 \right], \tag{5}$$

$\Psi(\mathbf{r})$ is the superconducting order parameter which is dependent on $\mathbf{r}$ but independent of τ, we have chosen various scales to make many couplings in (5) unity [16], $\mathbf{A}$ is the vector potential of the applied field, and $\kappa > 0$ is the repulsive coupling between the two orders. The action $S_\Phi + S_\Psi$ provides a theory of the SC to SC+SDW transition, including the ingredients for the repulsive interactions between the excitons and for the lowering of the exciton energy by the superflow.

In the context of the application to the recent STM measurements [4], a significant property of $S_\Phi + S_\Psi$ is that as long we are in the SC phase (which is evidently the case in [4]), not only do we have no static SDW order with $\langle \Phi_\alpha \rangle = 0$, but we also have $\langle \phi \rangle = \langle \Phi_\alpha^2 \rangle = 0$, and so there is no local static CDW order even in an external field, even though the energy of the spin/charge exciton has been considerably lowered. This is simply a consequence of the fact that all the terms in (3) and (5) are invariant under the sliding symmetry (4), and so the phase of the exciton has not been pinned. However, the presence of the vortices clearly breaks the translational symmetry on the lattice scale, and so the continuum theory should be supplemented by additional terms which implement this effect and pin the exciton;

a little thought using (1) shows that the simplest such term is

$$S_{\rm lat} = -\zeta \int d\tau \sum_{\mathbf{r}} |\Psi(\mathbf{r})|^2 \, \Phi_\alpha^2(\mathbf{r},\tau)\, e^{i2\mathbf{K}_s\cdot\mathbf{r}} + \text{c.c.} \tag{6}$$

where ζ is a new coupling constant. Because of the rapidly oscillating term, (6) will vanish in any region of space where $\Psi(\mathbf{r})$ is slowly varying. So the pinning of the exciton by (6) happens mainly in the vortex core (the diameter of the core is of the order of a couple lattice spacings), while the energy of the exciton is lowered by κ term in (5) by the superflow outside the vortex core. On long scales outside the vortex core it should be acceptable to replace (6) by

$$S_{\rm lat,1} = -\zeta_1 \int d\tau \, \Phi_\alpha^2(\mathbf{r}=0,\tau)\, e^{i\delta} + \text{c.c.} \tag{7}$$

for a vortex at $\mathbf{r}=0$, where the phase δ is determined by the microstructure of the vortex on the lattice scale. The term (7) breaks the symmetry (4), and so it is now possible to have static CDW order in the SC phase in an applied magnetic field. We still have $\langle\Phi_\alpha\rangle = 0$, but (7) does locally lift the 6-fold degeneracy of the exciton to 3+3. We can compute the static CDW order in the spirit of the calculation of [16], and in the Gaussian approximation to $S_\Phi + S_\Psi + S_{\rm lat,1}$, and to first order in ζ_1 we find for large $|\mathbf{r}|$

$$\left\langle \Phi_\alpha^2(\mathbf{r},\tau)\right\rangle = \left(\frac{3}{8\pi^{3/2} s_1^{1/4} c^{5/2}}\right) \zeta_1 e^{-i\delta} \frac{e^{-2r_1\sqrt{s_1}/c}}{r_1^{3/2}}, \tag{8}$$

where s_1 is the exciton "mass" s renormalized downwards by the superflow via the κ term in (5) (as in [16]), $c = (c_x c_y)^{1/2}$ and $r_1 = c\left((x/c_x)^2 + (y/c_y)^2\right)^{1/2}$; this implies a static CDW by (1) and (2). The length scale, $\xi_c = c/(2\sqrt{s_1})$, over which this CDW order appears has been significantly increased by the superflow around the vortex core *and* the exciton interactions $u_{1,2}$, while the order has been pinned by the vortex core via (7). In the absence of the pinning in (7) we would have $\langle\delta\rho(\mathbf{r},\tau)\rangle = 0$ in this SC phase.

3 Quasiparticle density of states

We now discuss the application of the above theoretical framework to the STM measurements in BSCCO of Hoffman *et al.* [4]. As we indicated earlier, they report observations of a modulation of period 4 in the local density of states (LDOS) in a small energy window around ± 7 meV in the superconducting region (with fully formed coherence peaks) outside the vortex core. Such a modulation can arise by scattering of the quasiparticles off either the SDW or the CDW correlations. The SDW order is dynamic and one of its effects will be an enhancement of the quasiparticle LDOS at energies large enough to allow the quasiparticles to decay by emission of a finite energy spin exciton. It remains to be seen whether the spin excitation spectrum of BSCCO in a magnetic field, as observed in neutron scattering experiments, has spectral weight at low enough energies for this effect to be important. We also note that the modulation in the LDOS will only arise as a consequence of the 3+3 splitting of the spin exciton by the potential in (6) or

(7). Here we only present our results for the simpler case of modulation induced directly by the CDW order; this order is made static by the pinning induced by the vortex cores (as in (8)), and can serve as an elastic scattering potential for the quasiparticles. The effect of an isolated elastic scattering potential in a d-wave superconductor has been well studied [26], and for large scattering a virtual bound state is formed at low energies; the effect of (8) can loosely be interpreted as a periodic version of this, with the weaker potential only leading to a periodic 'hump' or 'shoulder' in the quasiparticle LDOS.

This proposal immediately raises a puzzle which we have not fully resolved. In general, symmetry arguments indicate that the presence of the static CDW order in (8) implies that the quasiparticle LDOS should display a period 4 modulation at *all* energies, and not just on the sub-gap feature at ± 7 meV. A possible resolution of this puzzle is provided by an appeal to the effects of disorder: the signal-to-noise for any periodic modulation is largest at sub-gap energies, and that is where the CDW modulation is visible. At higher energies, random fluctuations in the background LDOS of the d-wave superconductor, and especially in the energy at which the coherence peaks are present, can mask the presence of a periodic modulation. A further consequence of our proposal is that the CDW order should be visible near any strong short distance imperfection which can provide a pinning potential as in (7), and not just near vortex cores.

As promised above, we conclude with a simple calculation of the effect of (8) on the LDOS. We diagonalized a d-wave BCS Hamiltonian on a square lattice,

$$H = \sum_{ij} \left(-t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \Delta_{ij} c_{i\sigma}^\dagger c_{j,-\sigma}^\dagger + h.c. \right) + \sum_i [v(\mathbf{r}_i) - \mu] c_{i\sigma}^\dagger c_{i\sigma} \,, \qquad (9)$$

where t_{ij} includes nearest-neighbor (t) and next-neighbor (t') hopping, μ is the chemical potential, the pairing amplitude Δ_{ij} is self-consistently determined from $\Delta_{ij} = V_{ij} \langle c_{i\sigma} c_{j,-\sigma} \rangle$, and V_{ij} is the nearest-neighbor pairing potential. The CDW modulation (1), (2), (8) is implemented via $v(\mathbf{r}) = v_1 \{\cos[\mathbf{K}_c \cdot (\mathbf{r} - \mathbf{r}_0)] + \cos[\mathbf{K}_c' \cdot (\mathbf{r} - \mathbf{r}_0)]\} \, e^{-|\mathbf{r}-\mathbf{r}_0|/\xi_c} \, (|\mathbf{r} - \mathbf{r}_0|^2 + 1)^{-3/4}$. In this initial calculation we did not include the usual modulation of the Δ_{ij} induced directly by the presence of the vortex: we expect this to be important only in the core of the vortex, whose physics we are not attempting to model here, and where the present BCS model is probably inadequate anyway. Fig. 1 shows a numerical result for the LDOS, integrated over an interval of sub-gap energies, obtained for a periodic 32×32 system with 20% (bulk) hole doping. The charge-density modulation caused by $v(\mathbf{r})$ clearly leads to a period-4 modulation of the sub-gap LDOS.

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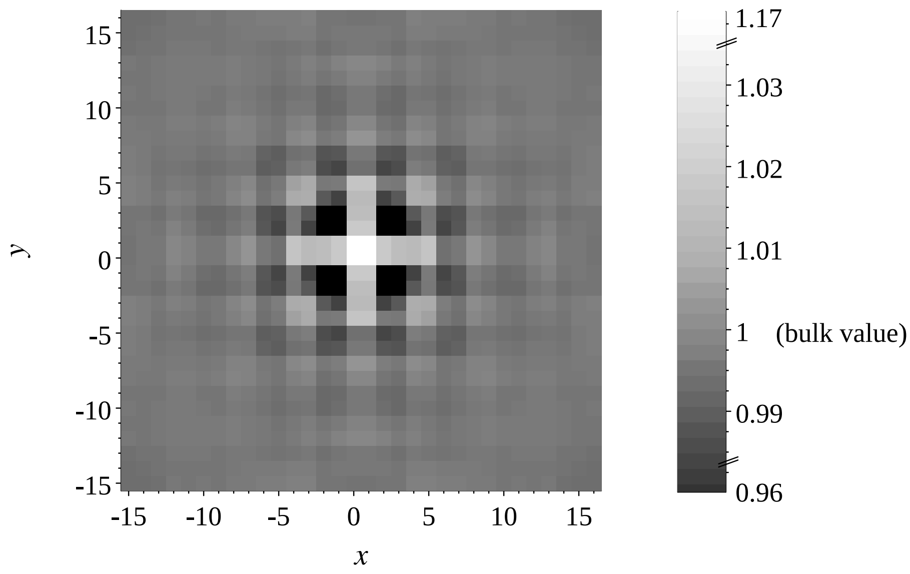

Figure 1. Grayscale plot of the CDW-induced quasiparticle LDOS, integrated over an energy interval $\Delta_0/10 \ldots \Delta_0/3$, where Δ_0 is the size of the bulk d-wave gap. The CDW modulation is plaquette-centered at (0.5,0.5), with wavevectors $\mathbf{K}_c = (\pi/2, 0)$ and $\mathbf{K}'_c = (0, \pi/2)$, decay length $\xi_c = 6$, and a strength $v_1 = t/5$. For computational reasons we have used a large pairing potential, $V = 2t$, but we do not expect qualitative changes for smaller V. A similar modulation is observed at the corresponding energy interval at negative energies.

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