Superconducting *d*-wave stripes in cuprates: Valence bond order coexisting with nodal quasiparticles

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We point out that unidirectional bond-centered charge-density-wave states in cuprates involve electronic order in both *s*- and *d*-wave channels, with nonlocal Coulomb repulsion suppressing the *s*-wave component. The resulting bond-charge-density wave, coexisting with superconductivity, is compatible with recent photoemission and tunneling data and as well as neutron-scattering measurements, once long-range order is destroyed by slow fluctuations or glassy disorder. In particular, the real-space structure of *d*-wave stripes is consistent with the scanning-tunneling-microscopy measurements on both underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ and $Ca_{2-x}Na_xCuO_2Cl_2$ of Kohsaka *et al.* [Science **315**, 1380 (2007)].

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I. INTRODUCTION

A remarkable aspect of the copper-oxide high-T_c superconductors is that various ordering phenomena apparently compete, including commensurate and incommensurate magnetisms, superconducting pairing, and charge-density-wave formation. (More exotic states have also been proposed, but not verified experimentally beyond doubt.) While commensurate magnetism and superconductivity are common phases in essentially all families of cuprates, the role of other instabilities for the global features of the phase diagram is less clear.

A particularly interesting role is taken by charge-density waves. Such states break the discrete lattice translation symmetry, with examples being stripe, checkerboard, and valence-bond order. In the compounds, $La_{2-x}Ba_xCuO_4$ and $La_{2-x}Sr_xCuO_4$ (with Nd or Eu codoping) evidence for stripe-like spin and charge modulations with static long-range order were detected,[1–4] in particular, near one-eighth doping. (This is supported, e.g., by strong phonon anomalies seen in neutron-scattering experiments.[5]) While in other cuprate families similar long-range order has not been found, signatures of short-range charge order, likely pinned by impurities, have been observed in scanning-tunneling microscopy (STM) on underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Refs. 6–9) and $Ca_{2-x}Na_xCuO_2Cl_2$.[9,10] The low-energy electronic structure in the presence of charge order turns out to be remarkable: In $La_{15/8}Ba_{1/8}CuO_4$, angle-resolved photoemission spectroscopy (ARPES) indicated a quasiparticle (QP) gap with *d*-wavelike form, i.e., charge order coexists with gapless (nodal) QP in the (1,1) direction [while antinodal QP near $(0,\pi)$ are gapped].[11] STM data on both underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ and $Ca_{2-x}Na_xCuO_2Cl_2$ and show QP interference arising from coherent low-energy states near the nodes, whereas electronic states at higher energy and wave vector close to the antinode are dominated by the real-space modulation of the short-range charge order.[7,9,12] This dichotomy in momentum space has also been found in ARPES experiments in $La_{2-x}Sr_xCuO_4$,[13] $Bi_2Sr_2CaCu_2O_{8+\delta}$,[14] and $Ca_{2-x}Na_xCuO_2Cl_2$ (Ref. 15) where well-defined nodal and ill-defined antinodal QP are frequently observed.

These results suggest that momentum-space differentiation and tendencies toward charge ordering are common to underdoped cuprates.[16–18] The concept of *fluctuating stripes*, i.e., almost charge-ordered states, has been discussed early on.[1,3,16,18,19] This concept, appropriate for compounds without static long-range order, assumes the existence of a nearby stripe-ordered state, with physical observables being influenced by the low-lying collective modes associated with charge-ordering instability. Following this idea, we have recently calculated[20] the spin excitation spectrum of slowly fluctuating (or disordered) stripes. We were able to show that fluctuating stripes give rise to an "hour-glass" magnetic spectrum, very similar to that observed in neutron-scattering experiments both on $La_{2-x}Ba_xCuO_4$ (Ref. 21) and $YBa_2Cu_3O_{6+\delta}$.[22,23]

The focus of this paper is on the electronic structure of stripe states. We introduce the concept of "*d*-wave stripes": Here, the modulation of charge densities has primarily a *d*-wave form factor, i.e., lives more on the bonds than on the sites of the square lattice, leaving nodal QP unaffected. We illustrate that a picture of such bond-centered charge order, coexisting with superconductivity (this state may be dubbed "valence-bond supersolid"), is consistent with various features seen in both ARPES and STM measurements. In particular, the real-space pattern of *d*-wave stripes (Fig. 1) is strikingly similar to the STM results of Ref. 9, obtained on underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ and $Ca_{2-x}Na_xCuO_2Cl_2$.

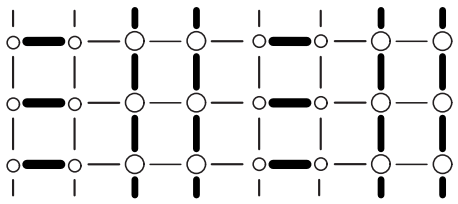

FIG. 1. Schematic real-space structure of a stripe state with primarily *d*-wave character and a 4×1 unit cell, i.e., $\mathbf{Q}=(\pm\pi/2,0)$. Cu lattice sites are shown as circles, with their size representing the on-site hole densities. The line strengths indicate the amplitude of bond variables such as kinetic and magnetic energies. The modulation in the site charge densities is small, whereas the one in the bond densities is large and of *d*-wave type (Ref. 24). Note the similarity of the bond modulation with the STM data of Ref. 9.

Other types of *d*-wave particle-hole order have been discussed before. (a) The *d*-density wave (or staggered-flux) phase[25] was proposed as a candidate for the pseudogap. However, it has no measurable charge modulation and shall not be discussed here. (b) Checkerboard (or plaquette) order[26,27] is related to stripes. While both can occur as stable phases (with similar energetics) in variants of the *t*-*J* model,[28,29] there are key experimental facts pointing toward stripe instead checkerboard order being the primary instability: (i) The STM data[9] clearly show that the rotation symmetry is locally broken from C_4 down to C_2. (ii) The momentum-space pattern of spin excitations arising from checkerboard order has been shown to be incompatible with the neutron response of materials such as $La_{2-x}Ba_xCuO_4$ or $YBa_2Cu_3O_{6+\delta}$.[20,30]

II. SUPERCONDUCTING VALENCE-BOND STATES

Numerous microscopic calculations, for Hubbard or *t*-*J* models at low doping, have indicated a tendency toward states with broken translational symmetry.[18,31–36] At low temperatures T, it is conceivable that this coexists with superconductivity.[28,36,37] In fact, such a scenario can be expected on general grounds: Upon destroying magnetic order in a square-lattice antiferromagnet (AF), paramagnetic states with valence-bond (or spin-Peierls) order are known to appear.[17] The introduction of charge carriers by doping then leads to superconductivity, coexisting with bond order for a finite doping range.[36,38] A global phase diagram has been worked out using a Sp($2N$) mean-field theory applied to the *t*-*J* model supplemented by longer-range Coulomb interaction:[36] At small doping, superconducting bond-centered stripe states occur, while homogeneous *d*-wave superconductivity is realized at larger doping. (Depending on microscopic parameters, the stripes may get replaced by checkerboard or spin-Peierls states.) Related superconducting charge-ordered states also appear in other theoretical treatments.[27,37]

Let us specify the various types of translational symmetry breaking on a square lattice, assuming the magnetic $SU(2)$ symmetry to be unbroken. (a) Spin-Peierls states have a 2×1 unit cell where all sites are equivalent, but the bonds are modulated. The C_4 rotation symmetry is broken; the ordering wave vector is $\mathbf{Q}=(\pi,0),(0,\pi)$. (b) Stripe states have a $N\times1$ unit cell ($N=4$ is particularly stable), both sites and bonds are modulated, $\mathbf{Q}=(\pm2\pi/N,0),(0,\pm2\pi/N)$, and C_4 is broken. (c) Checkerboard states have a $N\times N$ unit cell, both sites and bonds are modulated, $\mathbf{Q}=(\pm2\pi/N,\pm2\pi/N)$, but C_4 is intact. While stripe and checkerboard states can, in principle, be either site or bond centered, experimental evidence points toward bond-centered structures.[9,21,39]

In a quasiparticle picture, the symmetry-breaking orders can be translated into expectation values of fermionic bilinears: $\phi_1(\mathbf{k})=\langle c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow}\rangle$ captures homogeneous superconductivity, with $\phi_1(\mathbf{k})\propto\cos k_x-\cos k_y$ for *d*-wave pairing, while $\phi_2(\mathbf{k})=\langle c^\dagger_{\mathbf{k}+\mathbf{Q},\sigma}c_{\mathbf{k}\sigma}\rangle$ and $\phi_3(\mathbf{k})=\langle c_{\mathbf{k}+\mathbf{Q},\uparrow}c_{-\mathbf{k}\downarrow}\rangle$ originate from charge order. The directional dependence of $\phi_i(\mathbf{k})$ can be decomposed according to the representations of the point group. In the presence of unidirectional order, i.e., C_4 broken down to C_2, the *s*-wave and *d*-wave order parameters inevitably mix. Our superconducting stripe states below will have $\phi_{1,2,3}$ all nonzero. (Note that, e.g., ϕ_3 alone generates a Fulde-Ferrell-Larkin-Ovchinnikov state.)

III. *d*-WAVE STRIPES

Stripe states are best discussed in real space (phrased in the following for a square lattice of Cu atoms, keeping in mind that bonds of this lattice correspond to oxygen orbitals). Naively, the primary phenomenon of stripe order is a modulation of the on-site charge densities, $\langle c^\dagger_{i\sigma}c_{i\sigma}\rangle$, which translates into a momentum-independent (i.e., *s*-wave) order parameter $\phi_2(\mathbf{k})$. However, general arguments indicate[17,36] that the physics behind local ordering acts on bonds instead of sites: Stripe formation is driven by the competition between kinetic and magnetic energies, both living on lattice bonds. In such a bond-dominated stripe state, modulations in quantities like $\langle c^\dagger_{i\sigma}c_{i+\Delta,\sigma}\rangle$ can locally have different signs on horizontal and vertical bonds, implying a *d*-wave component of $\phi_2(\mathbf{k})$.

Given the mixing of *s*- and *d*-wave components, stripe states may have ordering primarily in either the *s*- or the *d*-wave channel. In the following, we shall argue in favor of stripes dominated by the *d*-wave component. Fourier transforming $\phi_2(\mathbf{k})$ into real space[24] leads to a stripe state as in Fig. 1—this is one of the main results of this paper. Importantly, the ordering pattern in Fig. 1 appears perfectly consistent with the STM data of Kohsaka *et al.* (Fig. 4 of Ref. 9), where locally well-formed period-4 structures are seen, consisting of distinct ladderlike objects.

Arguments in favor of stripes with a dominant *d*-wave component (Fig. 1) are as follows.[40] (i) Energetics: in the hole-poor regions, strong horizontal bonds form due to the tendency toward dimerization (i.e., optimizing the magnetic energy), whereas in the hole-rich regions, strong vertical bonds form optimizing the hole kinetic energy. (ii) Coulomb interaction disfavors on-site charge modulations and thus suppresses the *s*-wave component.

If stripe order coexists with superconductivity, then the bond pairing amplitudes, $\langle c_{i\uparrow}c_{i+\Delta,\downarrow}\rangle$, will be nonzero as well. Starting from a homogeneous *d*-wave superconductor, stripe order will induce a modulated *s*-wave pairing component, described by $\phi_3(\mathbf{k})$.

IV. MEAN-FIELD THEORY

Superconducting stripe states can be obtained in Sp($2N$) mean-field theory.[36] Consider an extended *t*-*J* Hamiltonian for fermions without double occupancies $c_{i\alpha}$, with spin $\alpha=1,\ldots,2N$ ($N=1$ is the physical value),

$$\mathcal{H}_{tJV}=\sum_{i>j}\left[-\frac{t_{ij}}{N}\sum_\alpha c^\dagger_{i\alpha}c_{j\alpha}+\text{H.c.}+\frac{V_{ij}}{N}n_in_j+\frac{J_{ij}}{N}\left(\mathbf{S}_i\cdot\mathbf{S}_j-\frac{n_in_j}{4N}\right)\right],\qquad(1)$$

with $n_i=\Sigma_\alpha c^\dagger_{i\alpha}c_{i\alpha}$. The spin operators $\mathbf{S}_i$ are fermion bilinears

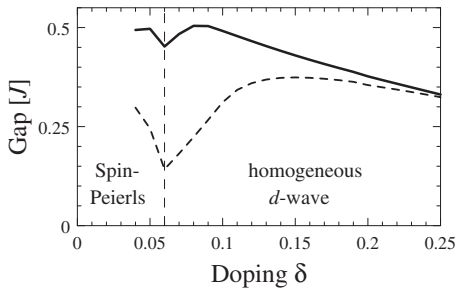

FIG. 2. Doping dependence of quasiparticle gap energies from Sp(2*N*) mean-field theory. The solid line shows the antinodal gap, i.e., the minimum QP energy along (k_x,π), for $t/J=4$ and $t'/t=-0.25$—here, only spin-Peierls order, but no stripes occur for doping $\delta>3\%$. (For stripe states, the characteristic gap scale is more difficult to extract due to band folding.) In addition, the dashed line shows the minimum QP energy along the boundary of the AF Brillouin zone (BZ) (Ref. 41).

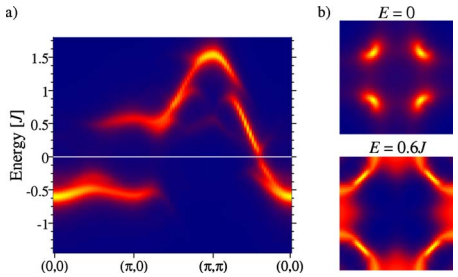

FIG. 3. (Color online) Electronic structure of a 4×1 stripe state from mean-field theory, here with $t/J=1.95$, $t'/t=-0.25$, overall doping $\delta=1/8$, and a hole distribution of 1.3:0.7 enforced by hand (see text). (a) Dispersion along high-symmetry lines in k space. (b) Constant-energy cuts through k space, showing nodal and antinodal structures. The spectra of horizontal and vertical stripes have been added, and an artificial broadening of $J/20$ was used.

times the traceless generators of Sp(2*N*). The fermion hopping t_{ij} will be nonzero for nearest and next-nearest neighbors, with values t and t', while the exchange J_{ij} is restricted to nearest-neighbor terms J. The average doping δ is fixed by $\Sigma_i\langle n_i\rangle=NN_s(1-\delta)$, where N_s is the number of lattice sites.

The spins and holes can be represented by auxiliary fermions $f_{i\alpha}$ and spinless bosons b_i, respectively, such that the physical electrons $c_{i\alpha}=b_i^\dagger f_{i\alpha}$. Via a Hubbard-Stratonovich decoupling of the AF interaction, we introduce link fields Q_{ij}, defined on the bonds of the square lattice. After taking the limit $N\to\infty$, the slave bosons b_i condense, $\langle b_i\rangle=\sqrt{N}b_i$, and the Q_{ij} take static saddle-point values. We are left with a bilinear Hamiltonian which can be diagonalized by a Bogoliubov transformation. At the saddle point, the slave-boson amplitudes fulfill $\Sigma_i b_i^2=N_s\delta$, and the link fields are given by $NQ_{ij}=\langle\mathcal{J}^{\alpha\beta}f_{i\alpha}^\dagger f_{j\beta}^\dagger\rangle$, where $\mathcal{J}^{\alpha\beta}$ is the antisymmetric Sp(2*N*) tensor. The distribution of the b_i is found be minimizing the saddle-point free energy, here the Coulomb repulsion V_{ij} enters (on a classical level only).

At nonzero doping and $T=0$, all mean-field phases are superconducting. At larger t/J, the on-site charge distribution is homogeneous except for tiny doping, but bond order of spin-Peierls type occurs at low doping. The doping dependence of the gap energy scale is shown in Fig. 2; it roughly follows the experimentally established pseudogap scale T^*.

At smaller t/J, stripe order occurs over a sizable doping range. As in most mean-field theories, the tendency toward ordering is overestimated: In a large parameter regime, the mean-field theory predicts bond-centered stripes with maximal charge inhomogeneity and strong bond order.[36] To obtain the electronic structure for a more realistic stripe state from the mean-field theory, we have employed the following modifications. (i) The distribution of on-site hole densities within the unit cell is enforced by hand through the b_i values. (ii) The parameter t/J is chosen such that the system is in the bond-ordered regime, but close to the transition to homogeneous superconductivity. These modifications anticipate that both quantum effects and Coulomb repulsion (beyond the classical approximation) reduce the amplitude of the charge modulations.[42] [Density-matrix renormalization group calculations for the 2*d t-J* model (with realistic t') showed signatures for bond-centered stripes with reduced on-site modulation amplitude.[34,35]]

A sample result for the electronic spectrum of a period-4 stripe state is shown in Fig. 3. In this calculation, the hole distribution was fairly inhomogeneous, $b_1^2=b_2^2=1.3\delta$, $b_3^2=b_4^2=0.7\delta$, and the link fields $|Q_{ij}|$ varied by a factor of 4 within the unit cell. Thus, the stripe state contained both sizable *s*- and *d*-wave components. Nevertheless, the spectrum is essentially gapless along the *k*-space diagonal, while a large gap appears near the antinodes (Fig. 3). This toy calculation illustrates a key point, namely, bond-centered stripe order is *compatible* with the presence of nodal quasiparticles, provided that the *s*-wave component of the order is not too large[43,44]—this compatibility was subject of discussions in the past.[45]

V. GLASSY DISORDER

Let us comment on the influence of quenched disorder arising from dopant impurities. In situations where a symmetry-breaking order is only "almost" static, adding disorder can pin the fluctuations and locally stabilize ordered islands. The result is a state with static short-range order, not unlike in glassy systems. For stripe order, this means that domains with segments of horizontal and vertical stripes will coexist, with a checkerboard structure of domain walls.[20,46] The electronic QP excitations now move in a static disorder potential, which couples strongly only to the QP near the antinodes, while nodal QP are little affected. As a result, the scattering rate along the normal-state Fermi surface will be strongly energy dependent, and gapless coherent nodal QP will coexist with incoherent antinodal QP.

Importantly, the disorder potential acts as a random *field* on charge stripes, smearing out any finite-temperature phase transition in the charge sector.[18,46] (This is distinct from the spin sector, where static order at low T is still accompanied by a sharp phase transition, as the disorder is of random-mass type.) At elevated temperatures, signatures of local valence-bond (i.e., singlet) formation will be visible below a temperature $T^*\sim J$ and will likely evolve continuously from

the high-temperature "pseudogap" scale to the low-temperature "superconducting" gap.

VI. THEORY VS EXPERIMENT

The described picture of valence-bond order, coexisting with superconductivity at low T, nicely ties in with various features of recent experimental data. (i) Models of coupled spin ladders, arising from bond-centered stripes,[47,48] provide an excellent description of the spin dynamics in stripe-ordered $La_{15/8}Ba_{1/8}CuO_4$.[21] (ii) The short-range charge order seen in STM on underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ and $Ca_{2-x}Na_xCuO_2Cl_2$ (Ref. 9) is bond centered and locally breaks the lattice rotation symmetry down to C_2. The glassy real-space structure is compatible with impurity-pinned short-range order, where fluctuations in the charge order parameter are primarily of phase instead of amplitude type.[20] (iii) The apparent d-wave gap of the nonsuperconducting stripe compound $La_{15/8}Ba_{1/8}CuO_4$ is naturally explained by d-wave stripes. (iv) To explain the absence of $3d$ superconductivity in $La_{15/8}Ba_{1/8}CuO_4$, "antiphase superconductivity" has been proposed.[49] This is similar to $\phi_3(\mathbf{k})$ above and broadly consistent with the picture advocated here.

VII. CONCLUSIONS

Building on earlier work on charge order in cuprates, we have pointed out that bond-ordered stripe states, possibly of glassy character and coexisting with superconductivity, provide a phenomenological framework which is consistent with many features of recent cuprate experiments. We believe that this strengthens the case for bond order (and associated local singlet formation) to be a common tendency in cuprates, likely relevant also for pseudogap phenomena. Let us note, however, that we think that stripelike translational symmetry breaking is a phenomenon *competing* with superconductivity, i.e., pairing is suppressed by stripes with spatial long-range order.

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