Stripe Formation by Long Range Interactions within SO(5) Theory

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We study the formation of stripe order within the SO(5) theory of high-T_c superconductivity. Spin and charge modulations arise as a result of the competition between a local tendency to phase separate and the long-range Coulomb interaction. This frustrated phase separation leads to hole-rich and hole-poor regions which are, respectively, superconducting and antiferromagnetic. A rich variety of microstructures ranging from droplet and striped to inverted-droplet phases are stabilized, depending on the charge carrier concentration. We show that the SO(5) energy functional favors nontopological stripes.

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One of the most striking features of the cuprates is the proximity between antiferromagnetic (AF) and superconducting (SC) phases as a function of doping. Recently it has been proposed that these two phases are unified by an approximate SO(5) symmetry [1]. A number of experimental consequences of this theory have been worked out [2–6]. Although SO(5) appears to be a natural framework for understanding the cuprates, no experiment has unequivocally tested the fundamental validity of the theory. One of its most direct predictions is the existence of a first-order transition from the AF to SC state as the chemical potential μ is increased beyond a critical value. However, this prediction is complicated by the fact that the doping x (not μ) is the experimentally tunable parameter. Experimentally, it is found that in the vicinity of the AF-SC transition, the cuprates show an increased sensitivity to disorder and inhomogeneity. In this Letter, we study this region of the phase diagram in the presence of the long-range Coulomb interaction within the SO(5) formalism and show how spatially inhomogeneous states can emerge.

In the $T - \mu$ phase diagram of SO(5) theory, there is a first-order line separating the AF and SC phases, across which the charge carrier density x jumps discontinuously. In the $T - x$ phase diagram, this translates into a two-phase region where AF and SC phases coexist. Phase separation into hole-rich and hole-poor regions was also noticed in studies of the t-J model [7,8]. However, as Emery and Kivelson [9] argued rather successfully, the long-range Coulomb interaction between charge carriers prevents macroscopic phase separation. The competition between the local tendency toward phase separation and the long-range Coulomb interaction leads to modulated domain structures at mesoscopic scales [10–13]. In the SO(5) theory, the hole-rich and hole-poor regions are, respectively, identified as having a superconducting and antiferromagnetic character. The spin and charge modulations of the system are interpreted as textures of the SO(5) superspin as it rotates in SO(5) space.

There is considerable evidence for modulated microstructure in the oxides. Domain formation has been reported in $La_{2-x}Sr_xCuO_4$ (LSCO) in muon spin resonance [14], NMR, and neutron diffraction experiments [15]. Neutron scattering measurements in $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ (LNSCO) provide direct evidence for stripe ordering in which the phase of the AF order shifts by π across a domain wall [16]. Furthermore, recent inelastic neutron scattering measurements in underdoped $YBa_2Cu_3O_{7-x}$ [17] and angle-resolved photoemission spectroscopy (ARPES) measurements in underdoped $Bi_2Sr_2CaCu_2O_{8-x}$ (BSCCO) [18] are not inconsistent with a striped phase interpretation.

In the mean field approximation of the SO(5) theory one minimizes the classical energy

$$H_1(n_a, p_a) = \frac{1}{4}\sum_{ab}\frac{L_{ab}^2}{\chi_{ab}} + g(n_1^2 + n_5^2) + \frac{\rho_s}{2}(\nabla\vec{n})^2 + E_c \qquad (1)$$

with $L_{ab} = n_a p_b - n_b p_a$ and constraints $n_a^2 = 1$, $n_a p_a = 0$. L_{ab} and $\vec{n}$ refer, respectively, to the SO(5) generators of rotation and the five-component superspin $\vec{n} = (\mathrm{Re}(\Delta), N_x, N_y, N_z, \mathrm{Im}(\Delta))$ [1]. The last term E_c is the Coulomb energy. Since, in SO(5) theory, the hole density is given by L_{15}, the charge density is $\rho(r) = L_{15}(r) - ex$, where ex is the charge of the neutralizing counterion charges which are assumed to be static and homogeneously distributed with a density x. We conjecture then that, if SO(5) theory is still valid in the presence of the long-range Coulomb interaction [19], the Coulomb energy in the mean field approximation will be given by

$$E_c = \frac{1}{2}\int\int \rho(r)V_C(r - r')\rho(r')\,dr\,dr'. \qquad (2)$$

It is important to emphasize that for homogeneous phases one recovers the basic SO(5) model because the

charge density vanishes exactly making the Coulomb interaction irrelevant. Hence the influence of the Coulomb term arises solely in the phase separation regime. Second, the assumption of immobile static counterions is known to fail for $La_2CuO_{4+\delta}$ [20]. In this case, the oxygen ions are mobile enough to screen the charge inhomogeneities which leads to macroscopic phase separation of superconducting and antiferromagnetic domains. This last fact provides strong evidence for the correctness of the SO(5) picture.

It can be proved that if H_1 is symmetric with respect to rotations within AF and SC subspaces ($\chi_{15} = \chi_s$, $\chi_{23} = \chi_{34} = \chi_{24} = \chi_a$, $\chi_{12} = \chi_{13} = \chi_{14} = \chi_{23} = \chi_{24} = \chi_\pi$), the minimal configuration has a form $\vec{n} = (n_1, n_2, 0, 0, 0) = (\cos\theta, \sin\theta, 0, 0, 0)$, $\vec{p} = (0, 0, 0, 0, p_5)$ and the constraints are automatically satisfied if we use the variables (θ, p_5).

With the addition of the long-range Coulomb interaction to the Hamiltonian, the behavior of the system is no longer tractable analytically and one must resort to numerical analysis. We note that a classical spin Hamiltonian

$$H_2 = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j - 2K \sum_i (S_i^z)^2 \tag{3}$$

can be transformed into the local part of H_1 by a Haldane map (see [21] for details). Here $J > 0$ and $K > 0$ are known functions of χ_{ab}, g, ρ_s. To match the whole expression (1) we add a term

$$V = \frac{1}{2} \sum_{i,j} \frac{(S_i^z - x)(S_j^z - x)}{\epsilon |\vec{r}_i - \vec{r}_j|}, \tag{4}$$

where ϵ is the dielectric constant of the material.

As emphasized earlier, since experiments are performed at constant carrier concentration, the Hamiltonian $E = H_2 + V$ is subject to the doping constraint $\langle S^z \rangle = x$. Numerically it is easier to study E than H_1 because the hole density is given explicitly by S^z rather than implicitly by L_{15}. The properties of E are studied using Monte Carlo simulations. In order to find the lowest energy state of the system, we perform simulated annealing from high temperature. We assume an $N \times N$ two-dimensional lattice where N can be up to 40 unit cells.

In the absence of the long-range Coulomb interaction, one can easily show that the system phase separates for densities x less than $x_c = K/(2J - K)$. The addition of the Coulomb term leads to a rich variety of modulated structures, which are shown on the phase diagram of Fig. 1. For large dielectric constant, three phases are found to be stabilized: a droplet phase made of SC droplets embedded in an AF background, a striped phase of alternating SC and AF stripes, and an inverted-droplet phase where the droplets are antiferromagnetic. Our numerical solutions (Fig. 2) show that the superspin stays in the AF or SC directions inside the domains and changes only in the thin domain walls. The structure represents a collection of solitons rather than a small modulation of the direction of $\vec{n}$. The superconducting density switches between 0 and x_c in AF and SC domains which means that the superconducting area fraction $A_{sc}/A = x/x_c$ leading to a linear relation between the superfluid density and the doping as seen in some experiments [22]. A simple physical argument for the pattern shape can be given in terms of interface energy [23]. As long as one of the phases (AF or SC) is in the minority, the energy of the AF-SC interface dominates over the Coulomb energy and circular domains are preferred as they minimize the length of this interface. However, the situation is reversed for $x \approx x_c/2$ where the repulsive interaction leads to dipole formation which favors elongated domains such as stripes.

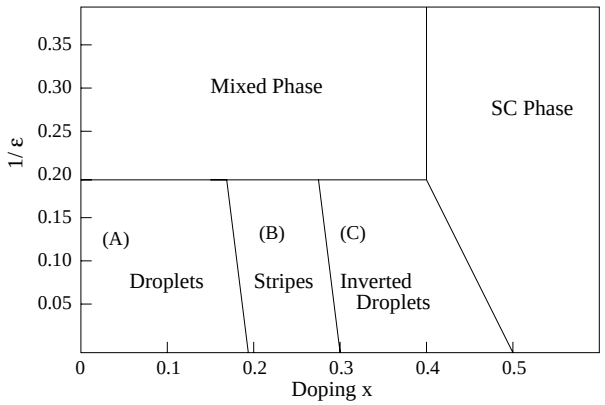

FIG. 1. Phase diagram as a function of strength of the Coulomb interaction $1/\epsilon$ and the hole density x for $K = 0.4$ and $J = 1$ which gives $x_c = 0.5$.

The striped phase is reminiscent of the domain structure observed in LNSCO, though the rows of charge are superconducting in our model. It is interesting to consider the superspin texture in the striped phases, namely, the relative phase shift of every other stripe. Numerically, it is found that the lowest energy states do not show any winding of the superspin in space. Hence, the phase of the AF order parameter does not shift by π on crossing a SC stripe. The same results were obtained for a simulation on a spin ladder where all configurations are necessarily one dimensional.

This absence of topological phase shift is in striking contrast to experimental data [16]; however, it can be proved analytically for the minimal periodic 1D configuration of (1) using the theorem of Pryadko *et al.* [24].

Theorem: For a functional

$$\mathcal{E} = \int \left(\frac{dv}{dr} \right)^2 + E_{\text{loc}}(v^2(r), r)\, dr + \int\int \rho(v^2(r), r) V(r - r') \rho(v^2(r'), r')\, dr\, dr' \tag{5}$$

of the function of one argument $v(r)$ the minimal configuration under a constraint $\int \rho(v^2(r), r)\, dr = 0$ does not cross zero.

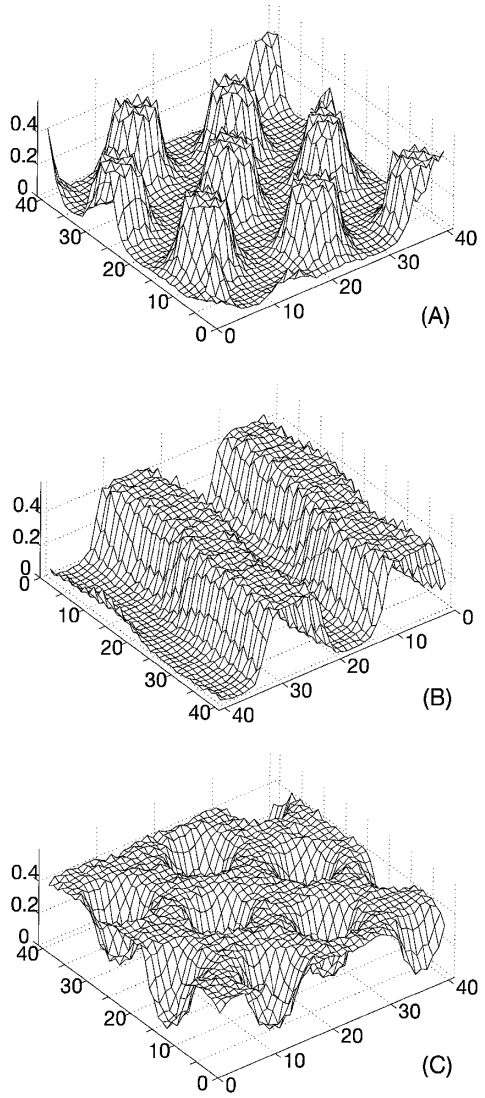

FIG. 2. Geometric phases as a function of doping: Hole density profile for the (a) droplet phase ($x = 0.12$), (b) striped phase ($x = 0.24$), and (c) inverted-droplet phase $x = 0.35$. The parameters chosen are $J = 1$, $K = 0.4$, and $\epsilon = 6$.

Applying it to (1) we note that as a function of θ both ρ and H_1 can be expanded in even powers around the points $\theta = 0, \pi$ and thus $\theta_{\min}(r)$ cannot cross these levels. In addition, let us perform a variable change $(\theta, p_5) \rightarrow (\theta, q = p_5/\cos\theta)$. Its Jacobian is sometimes infinite, but not on the minimal solution for which minimization of H_1 with respect to p_5 gives

$$p_5^{\min} = \frac{-\cos\theta}{\cos^2\theta/\chi_s + \sin^2\theta/\chi_\pi} \int V_C(r - r')\rho(r')\,dr'. \tag{6}$$

After the variable change $H_1(\theta, q)$ can also be expanded in even powers around the points $\theta = \pi/2, 3\pi/2$, so the minimal solution does not cross these levels either. Altogether, $\theta_{\min}(r)$ always stays in one of the four quadrants of the circle. For low dielectric constant, i.e., weak screening, we find that phase separation is precluded altogether. The system exhibits a homogeneous mixed phase in which the superspin points neither in the purely AF nor SC direction. This state is reminiscent of the putative supersolid phase in ^{4}He as both order parameters (AF and SC) are nonzero everywhere in the sample.

After the minimum of E is found, the chemical potential can be numerically calculated as $\mu = \partial E/\partial x$. As shown in Fig. 3, $\mu(x)$ becomes nonmonotonic and a region of $d\mu/dx < 0$ appears. Such a region is prohibited in thermodynamics, but in models with continuous charge density (as opposed to point charges) it is generic. The origin of the region in which the chemical potential is double valued is illustrated by Fig. 4. In the absence of Coulomb interactions and gradients the energy of a mixture with doping $x_{\min} < x < x_{\max}$ interpolates linearly between $E_{\min}$ and $E_{\max}$. The effect of Coulomb interactions and gradients is to increase the total energy of these intermediate states to $E_{\text{tot}}(x)$ as shown in Fig. 4. The dependence of μ on x is then given simply by $\mu = \delta E_{\text{tot}}/\delta x$, which is consistent with the numerical results of Fig. 3.

Because $E_{\text{tot}}(x_{\min,\max}) = E_{\min,\max}$ in models with continuous charge one has

$$\int_{x_{\min}}^{x_{\max}} (\mu(x) - \mu_c)\,dx = 0, \tag{7}$$

which applies beyond the SO(5) theory. Our numerical results are consistent with (7).

Experimentally, investigations of the chemical shifts in LSCO [25] and BSCCO [26] have shown that while the shift is large in overdoped samples, it is strongly suppressed and pinned in underdoped samples, in agreement with the phase separation picture. However, due to poor experimental resolution, it is not possible to ascertain the nonmonotonic behavior of $\mu(x)$. More experimental work is needed to test this prediction of our model. While this work was motivated by experiment, it should be emphasized that extensions of our model would be needed to make real contact with experiments. The lattice anisotropy of the cuprates will lead to an anisotropic

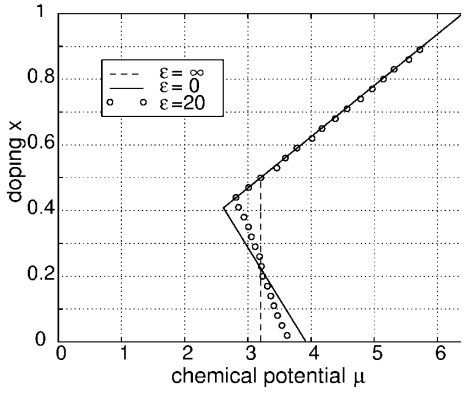

FIG. 3. x versus μ curve for three different values of ϵ, for parameters $J = 1$ and $K = 0.4$ which yield $x_c = 0.5$. The curves $\epsilon = 0$ (homogeneous) and $\epsilon = \infty$ (phase separation) are obtained from the analytic solution of Eq. (3). The circles are the data of the numerical solutions for $\epsilon = 20$.

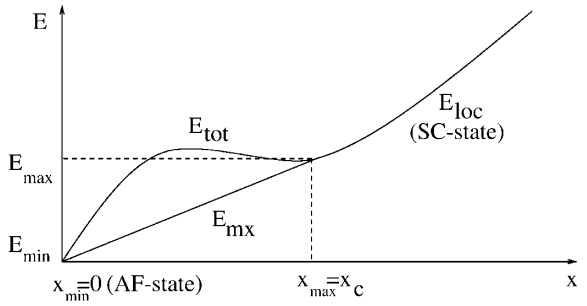

FIG. 4. State energy as a function of x: In the phase separation regime, the energy becomes a convex function of x.

AF-SC interface energy. We expect this anisotropy to enlarge the region of striped phase stability relative to that of the droplet phases, as the former can take best advantage of that anisotropy. Also, disorder will make the coefficients J and K (or χ_{ab} and g) and the charge of the counterions position dependent. Although the resulting effects are complex in character, we may speculate that for small disorder, the defects act as pinning centers for the stripes and lead to distortions of the domain structure as well as a loss of long-range order. This may explain the failure to observe droplet phases in the high-T_c superconductors. For strong randomness, the size of the domains would be predominantly set by the disorder instead of the long-range interactions [27,28]. However, we expect that the linear relation between the superfluid density and the doping should still hold in these glassy materials.

In summary, we have shown that the interplay between the long-range Coulomb interaction and the local tendency to phase separation of the SO(5) model leads to an interesting and remarkably rich phase diagram for the clean system. We found that the frustrated phase separation between hole-rich and hole-poor regions can provide an explanation for the gross features of the cuprates near the AF-SC transition when lattice anisotropy and impurity effects are taken into account. However, the SO(5) energy functional cannot have topological solutions as its lowest energy state. Therefore we believe that the topological nature of stripes that are observed in experiment must arise from microscopic properties of the coexisting states. Finally, we draw attention to the behavior of the chemical potential in the phase separation regime.

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