Nonuniversal Ordering of Spin and Charge in Stripe Phases

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We study the interplay of topological excitations in stripe phases: charge dislocations, charge loops, and spin vortices. In two dimensions these defects interact logarithmically on large distances. Using a renormalization-group analysis in the Coulomb-gas representation of these defects, we calculate the phase diagram and the critical properties of the transitions. Depending on the interaction parameters, spin and charge order can disappear at a single transition or in a sequence of two transitions (spin-charge separation). These transitions are nonuniversal with continuously varying critical exponents. We also determine the nature of the points where three phases coexist.

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High-T_c compounds fascinate not only because of superconductivity but also because of a variety of concurring orders. In particular, theoretical [1] and experimental [2] evidence has been found for stripes. Holes which are induced by doping condense into arrays of parallel rivers in the CuO_2 layers. Within a layer, each river acts as a boundary between antiferromagnetic domains with opposite sublattice magnetization. Thus, stripes are a combined charge- and spin-density wave.

Based on charge density and magnetization as order parameters, it is instructive to analyze the interplay of orders in the framework of a Landau theory [3]. However, in low dimensional structures fluctuations can be crucial for the nature of phases and of phase transitions. In particular, fluctuations play a central role (i) for spin-charge separation, i.e., the phenomenon that charge order emerges at higher temperatures than spin order (as observed in cuprates [4] as well as in nickelates [5]) and (ii) for the anomalous thermodynamic and transport properties of the cuprates near optimum doping [6]. To account for collective low-energy excitations of the electronic system, continuous deformations of perfect stripe order (spin waves or smooth stripe displacements) as well as topological defects (such as dislocations, vortices, or Skyrmions) must be considered. The latter were found to induce transitions between various liquid-crystal-like electronic phases [7]. Besides transitions which are related to a degradation of the charge and spin structure factors, Zaanen *et al.* [8] have suggested a further transition characterized by a less accessible, intrinsically topological order.

In this Letter we present a paradigmatic model which is amenable to a largely analytical analysis of the interplay between charge and spin orders. Motivated by the weakly coupled layered structure of the materials, we restrict our analysis to two dimensions. Since the relevant materials typically have a planar spin anisotropy, the out-of-plane component of the spins is neglected. Assuming quantum fluctuations to be weak in comparison to thermal fluctuations we treat all degrees of freedom as classical. In the framework of a renormalization-group approach we establish the phase diagram and the nature of the phase transitions. The latter are driven by three classes of topological defects (cf. Fig. 1): mixed defects combining a dislocation in the charge-density wave with a half vortex, charge loops (with a Burger's vector of two stripe spacings), and entire vortices [8].

We identify four different phases (cf. Fig. 2), depending on which types of topological defects proliferate. In phase I there are no free defects. In phase II only vortices are present, in phase III only charge loops are present, and in phase IV all types of defects are present. We characterize these phases by the range of charge order (CO), spin order (SO), and collinear order (LO). The phases are separated by transition lines along which the correlation functions decay with *nonuniversal*, continuously varying exponents. Slightly above the temperature T_{I} of the transition out of phase I, the short-ranged orders have a correlation length $\xi \sim \exp\{c(T-T_{\mathrm{I}})^{-\nu}\}$ with $\nu = \frac{1}{2}$ except for the triple points $P_{1,2}$ (cf. Fig. 2) with $\nu = \frac{2}{5}$.

To be specific, we assume that the stripes are parallel to the y direction with a spacing a. In the ground state, the charge density is modulated with a wave vector $\mathbf{q} = (2\pi/a, 0)$. In the absence of dislocations and loops, the stripe conformations can be described by a single-valued displacement field $\mathbf{u} \equiv (u, 0)$ and the domains between the stripes can be labeled by the step function $\theta(\mathbf{r}) \equiv \mathbf{q}\cdot[\mathbf{r} - \mathbf{u}(\mathbf{r})] + \sum_{m\neq 0} \frac{1}{im} e^{im\mathbf{q}\cdot[\mathbf{r}-\mathbf{u}(\mathbf{r})]}$, which increases by 2π across

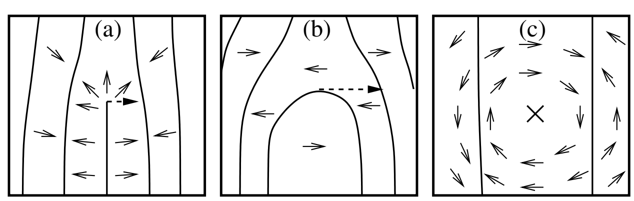

FIG. 1. Different types of topological defects in the charge-density (lines) and sublattice magnetization (bold arrows). (a) Combination of a stripe dislocation (dashed arrows correspond with the Burger's vectors) and a half vortex, (b) a charge loop, and (c) a vortex.

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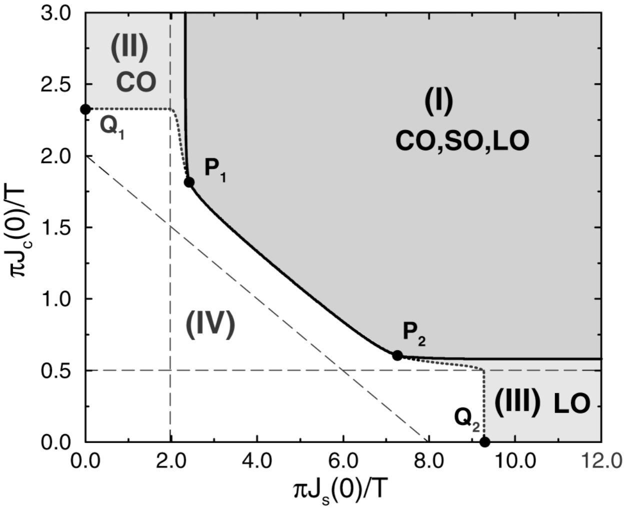

FIG. 2. Phase diagram. Thin dashed lines show where defects would become relevant for vanishing fugacities. For finite bare fugacities [9] the transitions are located at the bold lines. Phase I has no free defects and therefore CO, SO, and LO exist. In phase II, vortices proliferate and destroy SO. In phase III, free loops are present, destroying CO and SO. Eventually, all orders are absent in phase IV.

a stripe [at $x = na + u(\mathbf{r})$ with integer n]. The charge density is located at the domain boundary and can be expressed as $\rho(\mathbf{r}) = \frac{\lambda}{2\pi}\partial_x\theta(\mathbf{r})$, where λ denotes the charge per unit length per stripe. For XY spins $\vec{\sigma}(\mathbf{r}) \equiv \{\cos\Phi(\mathbf{r}), \sin\Phi(\mathbf{r})\}$, the magnetization (including the modulation by the antiferromagnetic order within the domains and by the antiphase boundary condition on the stripes) is captured by the angle $\Phi(\mathbf{r}) = \mathbf{Q}\cdot\mathbf{r} + \theta(\mathbf{r})/2 + \phi(\mathbf{r})$. Here $\mathbf{Q}$ is the antiferromagnetic wave vector and ϕ describes the smoothly varying spin Goldstone modes.

In the absence of topological defects low-energy excitations are wavelike and governed by the Hamiltonian

$$H_{\text{wave}} = \frac{1}{2}\int d^2r\{J_s(\nabla\phi)^2 + J_c(2\pi/a)^2(\nabla u)^2\} \quad (1)$$

with spin and charge stiffness constants J_α ($\alpha = \text{s, c}$). The structure factors $S_\rho(\mathbf{r}-\mathbf{r}') \equiv \langle\delta\rho(\mathbf{r})\delta\rho(\mathbf{r}')\rangle$ and $S_\sigma(\mathbf{r}-\mathbf{r}') \equiv \langle\vec{\sigma}(\mathbf{r})\cdot\vec{\sigma}(\mathbf{r}')\rangle$ decay algebraically, $S_\rho(\mathbf{r}) \sim \cos(\mathbf{q}\cdot\mathbf{r})r^{-\eta_\rho}$ with $\eta_\rho = 1/(2\pi K_c)$ and $S_\sigma(\mathbf{r}) \sim \cos[(\mathbf{Q}+\frac{\mathbf{q}}{2})\cdot\mathbf{r}]r^{-\eta_\sigma}$ with $\eta_\sigma = 1/(2\pi K_s) + 1/(8\pi K_c)$. We define the reduced stiffness constants $K_\alpha \equiv J_\alpha/T$.

In analogy to the Kosterlitz-Thouless (KT) transition [10], the presence of topological defects effects a screening of the stiffness constants. If neutral defect clusters unbind, these constants are renormalized to zero. For suitable values of the stiffness constants charge-loop pairs unbind as the only type of defects (phase III). Then *both* S_ρ and S_σ decay exponentially. To distinguish this phase from phase IV where all defects are free, an additional correlation function is necessary. For this purpose, Zaanen *et al.* [8,11] have suggested a highly nonlocal correlation function involving spin *and* charge. As a simpler and probably more physical alternative, we propose $C_\parallel(\mathbf{r}-\mathbf{r}') \equiv 2\langle(\vec{\sigma}_{\mathbf{r}}\cdot\vec{\sigma}_{\mathbf{r}'})^2\rangle - 1$ which measures the *spin collinearity* and has the advantage of being local and defined entirely in terms of spin variables. Collinearity is insensitive to continuous stripe displacements and to loops since the spin ground state remains collinear in the presence of such excitations. In the absence of topological defects in the spin sector (in phase I and III), spin waves lead to an algebraic decay of collinear order (LO), $C_\parallel(\mathbf{r}) \sim \cos(2\mathbf{Q}\cdot\mathbf{r})r^{-\eta_\parallel}$ with $\eta_\parallel = 2/(\pi K_s)$.

We now calculate the mutual screening of the defects which, in two dimensions, interact logarithmically on large distances. Therefore, their interactions can be captured by a Coulomb-gas formulation

$$H_{\text{top}} = \sum_{i\neq j}\sum_{\alpha=\text{s,c}} \pi J_\alpha m_{i\alpha}m_{j\alpha}\ln\frac{|\mathbf{r}_i - \mathbf{r}_j|}{a}, \quad (2)$$

for topological vector charges (m_{is}, m_{ic}) at positions $\mathbf{r}_i$. Additional core energies of such charges give rise to bare fugacities $y_i \equiv \exp\{-\pi C(K_s m_{is}^2 + K_c m_{ic}^2)\}$. C is a constant of order unity [9]. Vortices have a vector charge $(m_s, m_c) = (\pm 1, 0)$ and a fugacity $y_v = \exp(-\pi C K_s)$; loops are characterized by $(m_s, m_c) = (0, \pm 2)$ and $y_l = \exp(-4\pi C K_c)$. Dislocations have charges $|m_c| = 1$ and $|m_s| = \frac{1}{2}$ and fugacities $y_d = \exp\{-\pi C(K_c + K_s/4)\}$. Defects of higher charges are negligible for the critical aspects of the phase diagram.

We follow the renormalization approach developed by Kosterlitz and Thouless [10] for the usual scalar Coulomb gas and generalized to vector gases in the context of 2D melting [12]. The charges are assigned a hard-core cutoff a which is increased to $\tilde{a} = ae^{dl}$ under an infinitesimal coarse graining. Thereby, pairs of vector charges at a distance a annihilate each other if they have opposite charges; otherwise they recombine to a single nonvanishing vector charge. This coarse graining procedure leads to scale dependent stiffness constants and fugacities, for which we obtain the flow equations

$$\frac{dK_s^{-1}}{dl} = 2\pi^3(2y_v^2 + y_d^2), \quad (3a)$$

$$\frac{dK_c^{-1}}{dl} = 8\pi^3(2y_l^2 + y_d^2), \quad (3b)$$

$$\frac{dy_v}{dl} = (2 - \pi K_s)y_v + 2\pi y_d^2, \quad (3c)$$

$$\frac{dy_l}{dl} = (2 - 4\pi K_c)y_l + 2\pi y_d^2, \quad (3d)$$

$$\frac{dy_d}{dl} = \left(2 - \frac{\pi}{4}(K_s + 4K_c)\right)y_d + 2\pi(y_v + y_l)y_d. \quad (3e)$$

They have the symmetry $(K_s, y_v) \leftrightarrow (4K_c, y_l)$. A qualitative understanding of the phase diagram can be obtained from the rescaling contributions linear in the fugacities to the flow equations. Vortices proliferate for $\pi K_s < 2$ and loops for $4\pi K_c < 2$. Furthermore, for $\frac{\pi}{4}(K_s + 4K_c) < 2$ dislocations become relevant. The corresponding borders are shown in Fig. 2 as dashed lines.

In order to include the terms quadratic in the fugacities, the flow equations have to be integrated numerically. In phase I all fugacities tend to zero as $l \to \infty$ and K_s and K_c are renormalized to finite values $K_s(\infty)$ and $K_c(\infty)$ smaller than the initial ones. The defects can be considered as being bound in local clusters of vanishing total charge. Their fluctuations enhance the wave excitations such that CO, SO, and LO are quasi-long ranged: S_ρ, S_σ, and $C_\parallel$ decay algebraically as in the absence of defects. The exponents η are determined by the expressions given after Eq. (1) if the bare stiffness constants are replaced by the renormalized ones. Since the boundary of phase I flows to a line of fixed points (dashed lines in Fig. 2 for zero fugacities) with continuously varying values of the renormalized stiffness constants, the transition is nonuniversal with exponents given in Table I.

Outside phase I, at least one fugacity increases with the scale. Since our flow equations are valid only for small fugacities, they can be evaluated outside the ordered phase only up to a finite scale l^* where some fugacity becomes of the order of unity. The divergence of a fugacity drives one or both stiffness constants to zero. A divergence of the renormalized exponent η then signals short-ranged order with a finite correlation length, which scales as $\xi \simeq ae^{l^*}$ sufficiently close to phase I. Although the divergence of fugacities hints at the nature of phases II, III, and IV, the precise shape of these phases is determined by strong coupling (large fugacity) regimes beyond the validity of Eqs. (3).

In phase II, vortices proliferate and the spin stiffness K_s is renormalized to zero. This leads to a destruction of the spin and the collinear order, since the exponents η_σ and $\eta_\parallel$ are infinite. The corresponding correlation functions decay exponentially, $S_\sigma \sim C_\parallel \sim \exp(-r/\xi)$. Since K_s is renormalized to zero, the interaction in the spin sector effectively breaks down. Nevertheless, dislocations and loops are still coupled in the charge sector and can remain bound for sufficiently large K_c [13]. Then also charge order remains quasi-long ranged with finite η_ρ.

TABLE I. Values of the exponents η, ν at the phase transitions. Orders that become short ranged at a transition line (η jumps to infinity) are marked by an asterisk.

	CO	SO	LO	ν
I/II	$\eta_\rho \leq \frac{1}{3}$	$\eta_\sigma \leq \frac{1}{3}$ *	$\eta_\parallel = 1$ *	$\frac{1}{2}$
I/III	$\eta_\rho = 1$ *	$\eta_\sigma \leq \frac{1}{3}$ *	$\eta_\parallel \leq \frac{1}{3}$	$\frac{1}{2}$
I/IV	$\frac{1}{3} \leq \eta_\rho \leq 1$ *	$\frac{1}{6} \leq \eta_\sigma \leq \frac{1}{2}$ *	$\frac{1}{3} \leq \eta_\parallel \leq 1$ *	$\frac{1}{2}$
II/IV	$\eta_\rho = \frac{1}{4}$ *	$\eta_\sigma = \infty$	$\eta_\parallel = \infty$	$\frac{1}{2}$
III/IV	$\eta_\rho = \infty$	$\eta_\sigma = \infty$	$\eta_\parallel = \frac{1}{4}$ *	$\frac{1}{2}$
P_1	$\eta_\rho = \frac{1}{3}$	$\eta_\sigma = \frac{1}{3}$	$\eta_\parallel = 1$	$\frac{2}{5}$
P_2	$\eta_\rho = 1$	$\eta_\sigma = \frac{1}{3}$	$\eta_\parallel = \frac{1}{3}$	$\frac{2}{5}$

In phase III loop pairs unbind and the charge stiffness K_c is renormalized to zero, leading to $\eta_\sigma = \eta_\rho = \infty$ and therefore to a short-ranged spin and charge order. The spin order is destroyed because of the arbitrarily large fluctuations of the domain walls. Since K_s is screened only by bound vortices and dislocations, $\eta_\parallel$ remains finite and quasi-long-ranged collinear order is preserved. In phase IV the proliferating dislocations obviously render all correlations short ranged.

As pointed out above the precise location of transitions II/IV and III/IV cannot be obtained by the weak coupling (low fugacity) flow equations. Nevertheless, we now present qualitative arguments for their location, focusing on the example of transition II/IV. In the limit $K_s(0) = 0$ the interaction in the charge sector is simply switched off. Nevertheless, loops and dislocations interact in the charge sector, the former stronger than the latter. Therefore, the transition [point Q_1 with $K_c(\infty) = 2/\pi$] is driven by the unbinding of the dislocations. At this point loops are irrelevant and the transition belongs to the KT universality class. When the bare K_s is increased, it is renormalized to zero by free vortices and the transition occurs practically at the same value of K_c as long as $K_s \lesssim 2/\pi$. When K_s increases to the value where vortices start to bind, the transition line II/IV reaches the point P_1 at a smaller value of K_c since dislocations start to be stabilized by the additional interaction in the spin sector. The situation for the transition line III/IV is similar; in this case the interaction of the charge components of the mixed defects is screened by the proliferating charge loops.

At the triple points $P_{1,2}$ the critical properties are governed by the balanced competition between two types of defects which can recombine into each other. Therefore, these points do not belong to the universality class of the KT transition. Because of the symmetry of the flow equations we concentrate on point P_2. There one can neglect y_v to a good approximation and the conditions $y_l = y_d$ and $K_s = 12K_c$ (thin dotted line in Fig. 3 top) are conserved under the flow. In this case the flow equations for $Y := 2\pi\sqrt{6}y_d$ and the small variable $x := \frac{1}{\pi K_c} - 2$ read $\frac{dx}{dl} = Y^2$ and $\frac{dY}{dl} = xY + (1/\sqrt{6})Y^2$. Following Ref. [12], these differential equations can be solved analytically and result in a critical exponent $\nu = \frac{2}{5}$.

Thus, the exponent ν is discontinuous along the border of phase I. While this discontinuity describes the divergence of ξ in the thermodynamic limit, it is unlikely to be seen in samples of finite size. For large but finite system sizes, ξ appears to diverge with an effective exponent ν_{eff} which appears to vary continuously in the range $0.4 \lesssim \nu_{\text{eff}} \lesssim 0.5$. We have analyzed the divergence of ξ from a numerical integration of the flow equations up to $l_{\max} = 10^3$ which corresponds to astronomically large scales. The resulting ν_{eff} (cf. Fig. 3) shows a notch of a relatively small width which can become substantially larger for smaller values of $l_{\max}$.

From the phase diagram of our model several scenarios of spin-charge separation are possible. At low temperatures

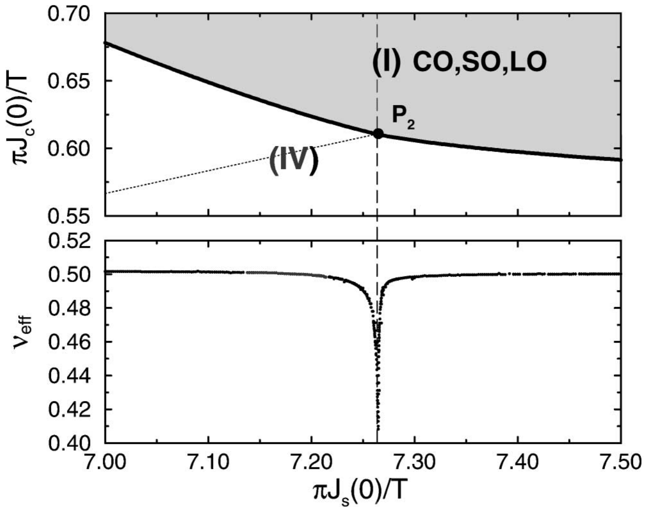

FIG. 3. Top: magnification of the phase diagram near point P_2. In this region, phase III is extremely narrow and masked by the transition line to the right of P_2. Bottom: Numerically calculated effective exponent ν_{eff} for $l_{\max} = 10^3$ along the boundary of phase I.

the stripe phase I is realized. (i) For $J_c > \frac{3}{4} J_s$, there occur *two distinct transitions* with increasing temperature: first into phase II (loss of SO and LO), then into phase IV (loss of CO). This scenario is observed in experiments [4,5]. (ii) For $\frac{1}{12} J_s < J_c < \frac{3}{4} J_s$ there is a *single transition* from phase I to phase IV where all orders disappear simultaneously. (iii) For $J_c < \frac{1}{12} J_s$, CO and SO disappear at the same temperature of the phase transition I/III, while LO disappears only at an even higher temperature at the transition III/IV. The ratio between J_s and J_c—which determines the scenario—can be tuned by doping. To establish the phase diagram in the doping-temperature plane one should know the dependence of the phenomenological constants J_α on these parameters. This dependence is not provided by our analysis. However, one can draw conclusions about J_α from a comparison of our phase diagram with experiments. For example, in a doping range where $T_{\mathrm{CO}} > T_{\mathrm{SO}}$, our analysis implies that $J_c > \frac{3}{4} J_s$ and that $J_c \sim T_{\mathrm{CO}}$. Furthermore, T_{CO} was found to have a maximum near a commensurate doping [4,5]. We interpret this as a maximum of J_c which could be enhanced by renormalization effects close to lock-in in a washboard potential.

In conclusion, we have examined a model for coupled spin and charge order in stripe phases. We have shown that the transitions between the various phases are nonuniversal. We have identified collinearity as a physical quantity that allows one to discriminate between phases III and IV. Several interesting questions invite future investigations, in particular, the properties of related quantum critical points at zero temperature and the influence of disorder (see also [14]) on the nature of ordering.

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