Charge Density Wave Formation in the Low-Temperature-Tetragonal Phase of Cuprates

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We calculate the influence of transverse fluctuations on the longitudinal dynamics in the striped phase of cuprates by using the bosonization technique. We find that a charge density wave instability can arise if the stripe is quarter filled and the underlying lattice potential has a zigzag symmetry. Our results explain why static stripes are experimentally observed in underdoped La$_{2-x}$Nd$_x$Sr$_2$CuO$_4$ exactly at the onset of the low-temperature-tetragonal transition.

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During the last years, a large number of experiments have confirmed the formation of 1D charge stripes in doped Mott insulators\cite{1,2}. Recently, it was shown\cite{2} that for La$_{2-x}$Sr$_x$CuO$_4$ co-doped with Nd the stripe structure becomes static and incommensurate peaks corresponding to charge- and spin-stripe order can be measured by quasi-elastic neutron scattering. Moreover, it was observed that for underdoped compounds ($x = 0.10$ and $x = 0.12$) the temperature $T_{co}$ at which charge order sets in coincides with the onset of a structural transition from a low-temperature-orthorhombic (LTO) to a low-temperature-tetragonal (LTT) phase, $T_{LT T}$, whereas for the optimally doped compound $T_{co} < T_{LT T}$\cite{3}. Therefore, although the formation of static stripes seems to be undeniably connected to the structural transition, it is not yet clear how and why this should happen, and moreover, why there is no correlation between $T_{co}$ and $T_{LT T}$ at optimal doping.

In this letter, we address these questions and show that a charge density wave (CDW) instability can arise if two conditions apply simultaneously, namely, if the stripe is quarter filled and the underlying lattice potential has a zigzag symmetry. This is the situation for underdoped cuprates in the LTT phase: neutron scattering experiments have shown that for (0.06 $< x < 0.12$) the stripes are incompressible, with one hole every two lattice sites\cite{4}. In addition, within the LTT phase the buckling of the oxygen octahedra has the zigzag symmetry needed to stabilize bond centered stripes. The consequence of the combined presence of both facts leads to the formation of longitudinal CDW if the transverse modes are frozen with a zigzag symmetry.

Before introducing our model of a Luttinger liquid coupled to transverse kinks, we briefly review the transverse dynamics of a chain of holes. This problem was considered by Zaanan et al.\cite{5}, who showed its equivalence to a quantum spin-1 chain. The full phase diagram for this problem was determined numerically by den Nijs and Rommelse\cite{6} after earlier calculations by Schulz\cite{7}, who treated the spin-1 problem as two coupled spin-1/2 chains. Here, we review Schulz calculations\cite{7} and generate the full phase diagram from this formalism. Then, we study the effect of a coupling between the longitudinal and the transverse sector to determine when the operator responsible for the CDW instability becomes relevant.

Our starting point for the transverse modes is the spin-1 Hamiltonian\cite{7}

$$H = \sum_n [-t (S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+) - J_z S_n^z S_{n+1}^z + d(S_n^z)^2].$$

By replacing the spin-1 operator by a sum of two spin 1/2 operators, $S_n = \tau_a(n) + \tau_b(n)$, performing a Jordan-Wigner transformation into a system of interacting fermions, and then using a standard bosonization technique, one finally obtains $H = H_+ + H_-$ with\cite{7}

$$H_+ = \frac{\mu_1}{\pi^2 \alpha^2} \int dx \left[ K_+ \pi^2 \chi_+^2 + K_-^1 (\partial_+ \Psi_+)^2 \right]$$
$$+ \frac{\mu_1}{\pi^2 \alpha^2} \int dx \cos \left[ \sqrt{2} \Theta_+ \right];$$

$$H_- = \frac{\mu_2}{\pi^2 \alpha^2} \int dx \left[ K_+ \pi^2 \chi_-^2 + K_-^1 (\partial_- \Psi_-)^2 \right]$$
$$+ \frac{\mu_3}{\pi^2 \alpha^2} \int dx \cos \left[ \sqrt{2} \Theta_- \right].$$

Here, $\Psi_{\pm} = (\Psi_a \pm \Psi_b)/\sqrt{2}$ and $\chi_{\pm} = (\chi_a \pm \chi_b)/\sqrt{2}$. The bosonic phase fields are

$$\Psi_{a/b}(x) = -\frac{i\pi}{\ell} \sum_{k \neq 0} \frac{1}{k} \left[ \tilde{\rho}_{R,a/b} + \tilde{\rho}_{L,a/b} \right] e^{-\alpha |k|/2 - ikx},$$

$$\tilde{\rho}_{R,L,a/b} = \frac{1}{\sqrt{2\pi}} \int_0^{\pi} dk \cos \left[ kx - \kappa \right] e^{-\alpha |k|/2}.$$

This model then reproduces the CDW instability observed experimentally. We calculate the influence of transverse fluctuations on the longitudinal dynamics in the striped phase. The longitudinal modes are described as Luttinger liquids. The coupling between the longitudinal and transverse modes arises because the electrons moving along the stripe are scattered from transverse kinks. By writing the Hamiltonian in a bosonic representation, we find several forward scattering channels and one $4k_F$ scattering momentum transfer from longitudinal to transverse modes. The latter becomes relevant at quarter filling and leads to the formation of a longitudinal CDW if the transverse modes are frozen with a zigzag symmetry.
where $\alpha$ is the lattice constant and $\ell$ the system size. The fields with different $a/b$ indices commute and $[\Psi_{a/b}(x), \Psi_{a/b}(y)] = i\delta(x-y)$. The $\Psi_{a/b}$ are related to density fluctuations of the $a/b$ fermions through $\partial_x \Psi_{a/b}(x) = -\pi[\hat{\rho}_{R,a/b}(x) + \hat{\rho}_{L,a/b}(x) - 1/2]$. The velocities of the acoustic excitations are $u_{\pm} \approx \pm t\sqrt{1+2(d-3J)/\sqrt{\pi t}}$ and $u_{\pm} \approx \pm t\sqrt{1-2(d+J)/\sqrt{\pi t}}$. Further, $K_+ = [1+2(d-3J)/(\pi t)]^{1/2}$ and $K_- = [1-2(d+J)/(\pi t)]^{1/2}$. The coupling constants for the non-linear terms are approximately given by $\mu_1 = \mu_2 = J_z + d$ and $\mu_3 = -t$. While the $\mu_1$ and $\mu_2$ terms represent, respectively, back- and forward scattering contributions, the $\mu_3$ term originates from a non-local Fermi coupling and is the so-called disorder operator. The most relevant operator resulting from the original Hamiltonian is $\cos(\sqrt{2}\Theta)$. There are other operators which mix the $(\pm)$ and $(\mp)$ sectors but their scaling dimension is such that they are never dominant.

To analyze the possible phases of the model defined through Eq. (1), we treat the non-linear terms as perturbations and consider their scaling behavior. The $\mu_1$ term is relevant for $d > 3J_z$. The transition at $d = 3J_z$ is the roughening transition of the string, which can be seen calculating the large $n$ behavior of the correlator of the transverse displacements $G_{a/b}(n) = \langle u(0)u(n) \rangle = \sum_{i,j=0}^{n-1} \langle S_i^z S_j^z \rangle$, where $S_i^z = u_{i+1} - u_i$. Using the bosonized form $S_i^z(x) \simeq -(\sqrt{2}/\pi)\partial_x \Psi_+ + (2/\pi\alpha)e^{i\pi x} \cos(\sqrt{2}\Psi_+) \cos(\sqrt{2}\Psi_-)$, we find the equal time correlation function $G_z = \langle S_i^z(0)S_i^z(x) \rangle \simeq (2K_+/\pi^2x^2) + C_ze^{i\pi x} |x|^{-2K_+/2K_-}$, which consists of a smooth and an oscillating part ($C_z$ is a constant). The smooth part gives rise to a logarithmic divergence of $G_a(n)$ for $K_+ \neq 0$. However, for $d > 3J_z$ the $\mu_1$ operator is relevant and $K_+$ scales to zero, killing the logarithmic divergence of $G_a(n)$.

The $(\mp)$ sector is more involved. The $\mu_2$ operator is relevant for $d + J_z < 0$ and $\mu_3$ is relevant for $d + J_z > -15\pi t/2$. Thus, the gaussian fixed point is never stable and the $(\mp)$ sector always flows to strong coupling. This implies that a perturbative approach starting from the Gaussian model cannot be trusted. However, it was pointed out by den Nijs that the $(\mp)$ sector has an Ising symmetry. It has a form identical to the continuum limit of a classical 2D XY model $H_{xy} = \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j)$ with a 2-fold (Ising) symmetry breaking term of the form $\cos 2\phi_i$. We therefore expect a transition in the $(\mp)$ sector of the Ising type. We locate the critical line of the transition as the line where the scaling dimensions of the two non-linear operators in $H_-$ are equal, $d + J_z \sim -3\pi t/2$.

To analyze the properties of the phases we investigate the behavior of the equal time correlation function $G_{\mp}(n) = \langle S^+(n)S^-(0) \rangle$. If $\Psi_+$ is ordered (i.e. $d > 3J_z$), then $G_{\mp}$ decays exponentially as $\Theta_+$ correlations are short ranged. Similarly, if $d < 3J_z$ and $d + J_z > -3t\pi/2$, such that $\Psi_-$ has long range order, then $\Theta_-$ correlations also are short ranged, again leading to an exponentially $G_{\mp}$. However, for $d < 3J_z$ and $d + J_z < -3t\pi/2$, $\Theta_+$ is ordered and $G_{\mp}$ decays algebraically, $G_{\mp}(x) \sim |x|^{-1/4K_+}$. Combining the results from the $(\pm)$ and $(\mp)$ sectors, we then find five different phases. 1) a gap-full flat phase, with dominant $\mu_1$ and $\mu_3$ perturbations, exponentially decaying $G_z$ and $G_{\mp}$ correlations and a finite limit of $G_u$. 2) A gap-less rough phase in which only $\mu_3$ is relevant, with an algebraic decay in the smooth part of $G_z$, exponentially decaying $G_{\mp}$ and logarithmically divergent $G_u$ correlations. 3) A gap-less bond centered (BC) rough phase with a zig-zag pattern (anti-ferromagnetic correlations with $S_z = \pm 1$ but no $S_z = 0$ states). This phase differs from the rough phase in that it has an algebraic decay in the $G_{\mp}$ correlations. 4) A BC flat phase with dominant $\mu_2$ and $\mu_3$ perturbations. Like the BC rough phase, this phase has a zig-zag pattern which now is however long ranged. This phase is gaped. 5) For $3J_z - d > \pi t/2$, the present analysis cannot be applied because the diagonalization of the quartic $a,b$ interactions through a Bogoliubov transformation breaks down, leading to an unphysical purely imaginary value of $K_+$. As argued by Schulz, this signals a transition to a ferromagnetic state, i.e. a diagonal stripe state.

Besides the five phases found by Schulz, den Nijs has identified a sixth phase, see Fig. 1. The additional phase found by den Nijs is a disordered flat phase (DOF), which is gap-full. This phase has, in contrast to the flat phase, a finite density of kinks and anti-kinks ($S_z = \pm 1$ states) but the $G_u$ correlator does not show a logarithmic divergence, making this phase different from the rough phase. In the DOF phase the kinks are positionally disordered, but have an anti-ferromagnet order in the sense that a kink $S_z = 1$ is more likely to be followed by an anti-kink $S_z = -1$ rather than another kink, with any number of $S_z = 0$ states in between them. In spin language, the DOF phase is the valence bond phase which is responsible for the Haldane gap.

In fact, there are signs of this transition also in the Abelian bosonization approach. At $d + J_z = 0$, $\mu_1$ and $\mu_2$ changes sign. This is unimportant for $\mu_2$ as in this parameter regime the $(\pm)$ sector is dominated by the $\mu_3$ and not the $\mu_2$ operator. However, if the $\mu_1$ operator is relevant, then a sign change of $\mu_3$ is of consequence. Typically, such a sign change is indicative of a competition between two fixed points. A similar situation occurs in a spin-1/2 chain with nearest and next-nearest interactions, where dimerized and anti-ferromagnetic ground states compete. In the present situation, the competition is between on-site $(d)$ and nearest neighbor interaction $(J_z)$. A useful order parameter to distinguish between the flat and the disordered flat phases is the parity of the steps, $P = \langle \cos(\pi u_n) \rangle$, which in bosonized form

\[ \chi_{a/b}(x) = \frac{1}{\ell} \sum_{k \neq 0} \left[ \hat{\rho}_{R,a/b} - \hat{\rho}_{L,a/b} \right] e^{-\alpha |k|/2 - ikx}, \]
becomes $P \sim \langle \cos[\sqrt{2}(\Psi_+(x) - \Psi_+(0))] \rangle$, with $x = 0$ being the boundary of the string. If the $\mu_1$ operator is relevant, the field $\Psi_+$ is pinned and a sign change in $\mu_1$ leads to a $\pi$ phase shift of $\sqrt{2}\Psi_+$. As a result, $P$ shifts from zero to a finite value (if the boundary term is left unchanged). Therefore, while the Abelian bosonization approach does not allow for a detailed study of the pre-roughening transition or the DOF phase, the existence of this transition can be readily inferred.

Physically, the coupling of the transverse and longitudinal modes arises from the scattering of the electrons which move along the stripe from transverse kinks. This interaction is local and we can express it in terms of the longitudinal electron density $\rho_{\uparrow/\downarrow}$ and the kink density $S_z^x$. We will consider only terms that couple the charge density to the kink density. Terms that couple the kinks and the spin density are irrelevant in presence of repulsive interactions and we thus omit them. A local coupling of the electron density to the kink density can thus be written as

$$H_{c1} = \gamma_1 \int dx (\rho_\uparrow + \rho_\downarrow) (S_z^x)^2$$
$$H_{c2} = \gamma_2 \int dx \rho_\uparrow \rho_\downarrow (S_z^x)^2$$  \hspace{1cm} (4)

with coupling constants $\gamma_1, \gamma_2$. These terms can be readily bosonized. From $H_{c1}$ one obtains the following terms,

$$H_{c1} \sim \int dx \partial_x \Phi_\rho \left[ \frac{2\gamma_1}{\alpha^2} \partial_x \Psi_+ + \lambda_1 \cos(\sqrt{2}\Psi_-) \right] + \lambda_2 \cos(\sqrt{2}\Psi_+) + \text{irrelevant terms,}$$  \hspace{1cm} (5)

with $\lambda_i = \gamma_i / (\sqrt{2}\pi^2\alpha^2)$. The first term represents forward scattering between the acoustic transverse and longitudinal charge modes. In general, these two modes have different velocities $u_+ \neq u_\perp$ and thus this interaction is retarded as can be seen by performing a Gaussian average over one of the modes. This first term and the Gaussian parts of $H_+ \cdot \Phi$ and $H_\rho$ can be jointly diagonalized, leading to a hybridization of the transverse and longitudinal modes. This leads to an instability of the system which is similar to the Wentzel-Bardeen instability in one dimensional metals coupled to phonons. However, this instability occurs only at a very large coupling $\gamma_1 \sim 4\sqrt{(\pi K_+ K_\perp) / (u_\perp u_\parallel)}$. For small $\gamma_1$, the case considered here, the zero momentum transfer interaction is not very efficient. Also, as the hybridization is small for small $\gamma_1$, the scaling analysis below is only weakly affected by the hybridization and we thus ignore this correction. The $\lambda_1$ and $\lambda_2$ terms are only important if the respective cosine terms have a finite expectation value. If they do, these terms act like a shift of the chemical potential of the electrons, as $\partial_x \Phi_\rho$ measures the deviation from the charge density of its equilibrium value. These terms compete however with terms generated by $\gamma_2$, as will be discussed below. Bosonization of the $\gamma_2$ interaction gives the following terms,

$$H_{c2} \sim \int dx \left[ \lambda_3 \partial_x \Psi_+ \cos(\sqrt{2}\Phi_\sigma) + \lambda_4 \cos(\sqrt{2}\Phi_\sigma) \times \cos(\sqrt{2}\Psi_-) + \lambda_5 \cos(\sqrt{2}\Phi_\rho - \sqrt{2}\Psi_+ + (4K_\perp - \pi) x) \times \cos(\sqrt{2}\Psi_-) \right] + \text{irrelevant terms}$$  \hspace{1cm} (6)
The $\lambda_1$ and $\lambda_3$ terms result from scattering involving two $a,b$ operators whereas $\lambda_3$ involves four $a,b$ operators. While the first two terms describe forward scattering, the $\lambda_3$ term results from processes with momentum transfer $4k_F$ from longitudinal to transverse modes. At $k_F = \pi/4$, i.e. at quarter filling of the stripe this term is important, as the oscillatory $x$ dependence vanishes.

To understand the effect of the longitudinal-transverse coupling we examine the scaling dimensions of the $\lambda_i$ operators. We envision strongly repulsive interactions among the electrons on the stripe with $K_\rho < 1$ and $K_\sigma > 1$. The $\lambda_4$ operator is relevant only for $K_\sigma + K_+ < 1$ and thus unimportant. Similarly, $\lambda_3$ can be neglected as it is relevant only for $K_\sigma < 1/2$. The $\lambda_1$ operator is relevant for $K_- < 1/2$, $\lambda_2$ is relevant for $K_+ < 1/2$ and the $\lambda_5$ operator is relevant for $2K_\rho + K_+ + K_- < 2$.

Let us consider that $K_+ < 1$, i.e. the (+) sector is massive. In that case, the transverse modes behave at large wavelengths as if $K_+ = 0$. Then, if $2K_\rho + K_+ < 2$, the $\lambda_5$ operator will become relevant at large scales. The $\lambda_3$ term pins the longitudinal charge modes to the transverse modes and induces a longitudinal CDW. This is seen for the case with $K_- < 1/2$, i.e. in the BC flat phase, where both $\Psi_+$ and $\Psi_-$ have long range order. The freezing of the transverse modes in a zig-zag pattern leads to a $\pi$ periodic potential for the transverse modes and allows for Umklapp scattering of the charge sector, thus unimportant. Similarly, similarly a relevant $\lambda_5$ term pins the transverse charge modes to the longitudinal modes.

In conclusion, we evaluated the effect of transverse fluctuations on the longitudinal transport in a Luttinger liquid stripe phase. We found that a CDW instability arises if the stripes are quarter filled and the underlying potential has a zigzag symmetry. Our results explain why static CDWs are formed in under-doped cuprates exactly at the onset of the LTT structural transition.

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