Melting of the stripe phases in the $t$-$t'$-$U$ Hubbard model

Marcin Raczkowski, a,b,1 Raymond Fréard, a,* Andrzej M. Oleś b

Abstract

We investigate melting of stripe phases in the overdoped regime $x \geq 0.3$ of the two-dimensional $t$-$t'$-$U$ Hubbard model, using a spin rotation invariant form of the slave boson representation. We show that the spin and charge order disappear simultaneously, and discuss a mechanism stabilizing bond-centered and site-centered stripe structures.

Key words: doped cuprates, charge order, stripe phase

PACS: 74.72.-h, 71.45.Lr, 75.10.Lp

It is now well established that the doped cuprates show many highly unusual properties both in normal and superconducting state. Among them, stripe phase, discovered in theory [1] and confirmed by experiment [2], attracted a lot of interest. Instead of moving independently, the holes introduced to an antiferromagnetic (AF) Mott insulator self-organize either on site-centered (SC) nonmagnetic domain walls (DW) separating AF spin domains, or on bond-centered (BC) DW made out of pairs of ferromagnetic spins [2]. Such a tendency towards phase separation is fascinating, and offers a framework for interpreting a broad class of experiments, including the pseudogap at the Fermi energy observed in the angle-resolved photoemission (ARPES) spectra of La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) for the entire underdoped regime ($0.05 \lesssim x \lesssim 0.125$), reproduced within the $t$-$t'$-$U$ Hubbard model [3]. Therefore, we argue that this model is sufficient to investigate generic features of stripe phases.

Two main scenarios for a driving mechanism of the stripe phase have been proposed [4]. In the first one stripes arise from a Fermi surface instability [1]; then spin and charge order simultaneously, or charge order follows spin order. The second scenario comes from Coulomb-frustrated phase separation suggesting that stripe formation is commonly charge driven, and the charge order sets in first when the temperature is lowered. However, slave boson studies of the two-dimensional (2D) $t$-$t'$-$U$ Hubbard model showed that the spin susceptibility diverges while the charge susceptibility does not [5], so the microscopic origin of the stripe instability is unclear.

We investigate the mechanism leading to phase separation and the melting of vertical BC and SC stripe phases in the overdoped regime ($x \geq 0.3$, where $x = 1 - n$ and $n$ is an average electron density per site) of the 2D $t$-$t'$-$U$ Hubbard model. We employ the spin rotation invariant slave boson (SB) representation of the Hubbard model [6], and perform the calculations on larger (up to $144 \times 144$) clusters than those studied recently [7]. This allows one to obtain unbiased results at low temperature $T = 0.01t$.

For the model parameters for LSCO: $U/t = 12$ and $t'/t = -0.15$, we obtain that the most stable SC stripes are separated by $d = 4$ lattice spacings at dopings $0.124 \lesssim x \lesssim 0.2$ ($0.2 \lesssim x \lesssim 0.34$), respectively. As shown in Fig. 1(a), increasing doping stabilizes the SC stripes with a single atom in the AF domains. Also for the BC stripes the size of the AF domains decreases with increasing doping, varying from $d = 5$ ($0.10 \lesssim d \lesssim 6$) at $x = 0.124$ to $d = 4$ ($0.33 \lesssim x \lesssim 0.34$) at $x = 0.34$. It has been checked that the ratio of the BC stripe size to the SC stripe size is independent of doping.
x \leq 0.13) through d = 4 (0.13 \leq x \leq 0.19) and down to d = 3 at higher doping, as there is no BC configuration with d = 2. For both types of stripes, the distance between them is locked to four in a sizeable doping range above x \approx \frac{1}{4}, in agreement with neutron scattering experiment \cite{8} and with theory \cite{3} for LSCO.

In Fig. 1(a) we show the energy gain of the stripe phases with respect to the paramagnetic phase $\delta F$. Remarkably, the difference in energy between the best SC and BC stripes is smaller than both the accuracy of the calculations, and the resolution of Fig. 1(a), suggesting that quantum fluctuations might be important. We characterize the melting of stripes by their SB local averages: density $n_i = \sum_{\sigma} \langle n_{i\sigma} \rangle$, magnetization $m_i = \langle \sigma_i \rangle$, and double occupancies $D_i = \langle n_{ii} \rangle$.

In the $d = 2$ SC stripe, reported here for the first time, the two $\delta n_i(x)$ curves are symmetrical in Fig. 1(b). In contrast, in the $d = 3$ BC stripe there are two sites with weak magnetic moments per one strongly polarized site. We note that, unlike in the SC phase, the variation in density is largest on the strongly polarized sites in the BC phase. The magnetic moments $m_i$ vanish for both types $d = 3$ stripes at the same doping $x = 0.375$ [Fig. 1(c)], suggesting that they originate from the same instability.

The microscopic mechanism stabilizing the $d = 2$ SC stripes appears to differ markedly from the one stabilizing the $d = 3$ ones \cite{9}. For $d = 2$ [Fig. 1(d)], the reduction of double occupancy is strongest on the magnetic sites, and the corresponding reduction of interaction energy is larger than the gain of free energy [see Fig. 1(a)]. Thus the mechanism leading to the formation of the $d = 2$ stripe is primarily local, making use of two complementary effects helping to reduce double occupancy: finite magnetization at magnetic sites and reduced electron density at nonmagnetic ones. Even though such a state loses kinetic energy, the gain in the interaction energy overcompensates this loss, stabilizing this order in a wide doping range $x \leq 0.485$.

In contrast, for $d = 3$ stripes, both contributions to the free energy are substantially decreased while stripe order starts melting already at $x < 0.3$ mainly by faster removing double occupancies from the stripe DW than from AF domains leading to gradually disappearing magnetic moment upon doping. Therefore, both potential and kinetic energy (including the superexchange) cooperate to stabilize stripes with $d > 2$. In fact, for both $d = 3$ stripes, the mechanism is doping dependent. In the small magnetization regime, the interaction energy plays the leading role. However, under a further decrease of hole density, this gain nearly saturates (at $x \approx 0.33$), and the gain in the kinetic energy starts to dominate. Moreover, it is only slightly larger for the SC stripe compared to the BC one, and therefore it is easily compensated, mainly by the presence of finite magnetic moments at BC domain walls.

As a common feature, the spin and charge order disappear at the same critical doping. Therefore, in the absence of longer ranged Coulomb interaction the charge order is always accompanied by the spin order.

Summarizing, we have investigated the microscopic mechanisms responsible for the formation of the vertical BC and SC stripes in the extended 2D Hubbard model. Interestingly, we found that BC and SC stripes remain nearly degenerate, and both spin and charge order vanish simultaneously when they melt, demonstrating a cooperative character of the stripe order.

References

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