Partially filled stripes in the two dimensional Hubbard model: statics and dynamics

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The internal structure of stripes in the two dimensional Hubbard model is studied by going beyond the Hartree-Fock approximation. Partially filled stripes, consistent with experimental observations, are stabilized by quantum fluctuations, included through the Configuration Interaction method. Hopping of short regions of the stripes in the transverse direction is comparable to the bare hopping element. The integrated value of $n_k$ compares well with experimental results.

By now it is well established that charged stripes are formed in a significant doping range of cuprate oxides. The existence of these stripes was predicted, on the basis of mean field calculations, in advance of its observation, both in the one and the three bands Hubbard model. This is one of the scarce theoretical results in the field of high-Tc superconductivity which was confirmed after its prediction. Interest in these calculations decreased, as it was generally understood that the Hartree-Fock approximation was unable to obtain the partially filled stripes observed experimentally. Unrelated calculations found stripes with different fillings in the t-J model, and, using different techniques, in the Hubbard model, although other numerical calculations show conflicting results. Alternatively, it has been argued that stripes in doped Mott antiferromagnets arise from a tendency towards phase separation, frustrated by electrostatic interactions. Stripes in the Hubbard model have also been analyzed within slave-boson techniques, which use the Hartree-Fock solutions as input.

In the present work we show that the mean field calculations, initially used to demonstrate the existence of stripes, can be systematically improved in order to study the partially filled stripes observed experimentally. In addition, they provide significant insight into the internal structure of the stripes and their fluctuations in the transverse direction. The Hartree-Fock method can be considered a quasiclassical approximation to the spin and charge degrees of freedom. Their low amplitude quantum fluctuations can be incorporated by using the Random Phase Approximation. In addition, one needs to consider quantum tunneling processes between degenerate, or nearly degenerate, Hartree-Fock solutions, when there are many. This is achieved with the Configuration Interaction method (CI), widely used in quantum chemistry. The combination of the Hartree-Fock and CI methods gives reasonable results even when applied to one dimensional systems. The CI method restores the symmetries broken by the Hartree-Fock approximation, and provides information on the quantum dynamics of the static solutions obtained in mean field, which can be broadly classified into spin polarons or stripes.

Previous mean field studies have focused on filled stripes, which tend to be the solutions with the lowest energy per hole in this approximation, especially for the values of $U/t \sim 4$ used in the initial studies. There are, however, self consistent solutions which describe partially filled stripes. These solutions have energies per hole comparable to those of the filled stripes for $U/t \sim 8 - 20$.

Typical stripe solutions obtained in this work within the mean field approximation and periodic boundary conditions, are shown in Fig. 1, where, for simplicity, we show results obtained in a $5 \times 4$ cluster, and $U = 8$ (hereafter we shall use $t$ as the unit of energy). The filled stripe, like the ones considered in previous mean field calculations, is shown in Fig. 1 c), while Fig. 1 a) and b) correspond to half filled stripes, not reported earlier. These textures correspond to self consistent Hartree Fock solutions, and can be found in clusters of any size. A generalization of the solution shown in Fig. 1 b) to a $16 \times 16$ cluster with 1/8 holes per site (32 holes) is shown in Fig. 2. We have also calculated the energy required to create a hole in these configurations. In order to subtract the energy of the antiferromagnetic background we have averaged the energy per site obtained on $4 \times 4$, $4 \times 6$ and $6 \times 6$ clusters, the result is 0.463 per site. The so obtained energies per hole are reported in Table I. It is interesting to note that the standard solution for the filled stripe shown in Fig. 1 c) is the best UHF solution only for sufficiently small $U$, while at intermediate $U$ (including the case of $U = 8$ discussed here), there are better solutions which are inhomogeneous along the stripe direction, with $\epsilon_{HF} = -1.081 t$, slightly smaller than the energies of the half-filled stripes. We also show in Table I the energy gain due to hybridization with displaced solutions of the same type ($\epsilon_{CI}^0$).
FIG. 1. Spin and charge textures for the three stripe solutions discussed in the text. Solutions a) and b) correspond to half filled stripes, while solution c) is a filled stripe.

| Half filled stripe | Half filled stripe | Filled stripe |
|--------------------|--------------------|--------------|
| $\varepsilon_{HF} = -0.959t$ | $\varepsilon_{HF} = -0.991t$ | $\varepsilon_{HF} = -0.958t$ |
| $\varepsilon_{CI} = -1.47t$ | $\varepsilon_{CI} = -1.12t$ | $\varepsilon_{CI} = -1.36t$ |

Table I. Energies, per hole, of the stripe solutions shown in Fig.[1]

The best energies per hole that we have obtained, after combining, within the CI scheme, the previous configurations and others not shown in Fig.[1], are $\varepsilon_{CI} = -1.573t$ (half filled stripes) and $\varepsilon_{CI} = -1.364t$ (filled stripes).

The results in Table I have been obtained for a single stripe. They have uncertainties due to the cluster size dependence and the subtraction of the antiferromagnetic background. In general, the energy differences are small, of a few hundredths of $t$. The stabilization of half filled stripes seems to be a general result, at least for values of $U/t$ in the range 6-20. The value $U/t = 8$ corresponds to a $t$-$J$ model with $J/t = 1/2$. The energy per hole that we obtain compares well with calculations for this model [20]. For $U/t = 12$ ($J/t = 1/3$), we obtain $\varepsilon_s \approx -1.71 \pm 0.05t$. This value is also in reasonable agreement with other calculations [21].

We have also calculated the hole-hole correlation, $C_{i,j} = \langle (1 - n_i)(1 - n_j) \rangle$ for the half-filled stripe in a 5 × 4 cluster. The optimal CI wavefunction, discussed above, was used in the calculation. $C_{i,j}$ shows a maximum (0.021) when the holes are separated by a vector $r_{ij} = r_i - r_j = (0, 2)$, that is when they are two lattice constants apart along the stripe direction. This feature of the hole-hole correlation differentiates stripes from other two hole configurations investigated within the $t$–$J$ [22] or the Hubbard models [23][24]. We note, however, that $C_{i,j}$ is also rather large (0.011) for the hole-hole separation at which the results reported in those studies show the maximum hole-hole correlation, namely, $r_{ij} = (1, 1)$.

Our method is well suited to analyze quantum fluctuations of stripes in the transverse direction, as we can calculate the off diagonal terms of the full hamiltonian between stripe solutions which are displaced by an arbitrary lattice constant. We find that the matrix element which describes the shifting of a stripe segment of length $l$ by one lattice unit decays as $t_s e^{-l/l_0}$, where $t_s \sim t$ and $l_0 \sim 2$.

Note that the two main configurations involved, Fig.[1] a) and b), can be viewed as a superposition of site centered and bond centered one dimensional domain walls [19]. These configurations lead to a very accurate description of the dynamics of a hole in the one dimensional Hubbard model [13]. The fact that the maximum hole-hole correlation is found along the stripe (see discussion above) implies an additional similarity between the stripe solution and one dimensional Luttinger liquids. Thus, the stripes can be viewed as a one dimensional system at quarter filling.
Because of the commensuration with the lattice, we find a gap in the charge spectrum. We estimate the value of this gap, $\Delta_{ch}$, beyond mean field theory, by calculating $\Delta_{ch} = E_{n_h+1} + E_{n_h-1} - 2E_{n_h}$, around the optimal filling. We obtain, for $U/t = 8$, $\Delta_{ch} = 0.7 \pm 0.1t$, which is lower than the Hartree-Fock gap. For $U/t = 12$, we find $\Delta_{ch} = 0.5 \pm 0.1t$, which compares well to the gap obtained using dynamical mean field techniques [10].

Upon doping, we expect that each electron leads to two charge 1/2 solitons [24]. The Hartree-Fock method is well suited to visualize charge fractionalization of this type [25], as shown in Fig. [3 a)]. The fact that the stripe is embedded in a two dimensional background allows for an alternative solution, the step [26], also shown in Fig. [3 b)]. This solution has a slightly lower energy. Thus, we expect that deviations from half filling in the stripes will lead to the formation of steps. We can calculate the quantum dynamics of the steps along the direction parallel to the stripe. Within the CI method, a step like the one shown in Fig. [3 b)] gives rise to a band of delocalized states of width $0.59t$ ($U/t = 8$) and $0.37t$ ($U/t = 12$). This bandwidth measures directly the delocalization of the step along the stripe due to quantum fluctuations. The energy gain due to this hybridization, $0.29t$ ($U/t = 8$) and $0.18t$ ($U/t = 12$), further stabilizes the step.

The formation of steps is hindered when the stripes are sufficiently close. Experiments suggest that the closest distance between stripes is four lattice units, which is realized at 1/8 doping [27]. Near this filling, holes in the stripes will give rise to charge fractionalization and Luttinger liquid behavior [28,29].

We have also computed the value of $n_{k}$, from the solutions described above. They are shown in Fig. [4], calculated in a 16 × 16 cluster, and obtained by integrating in energies over the top half of the valence band and the stripe states induced within the gap. Note that the charge and spin distributions are homogeneous in real space, as the CI method restores full translational symmetry. The strong anisotropy, in $k$ space, of $n_{k}$ reflects the existence of the stripe (see also [30,31]), and is consistent with the experimental results reported in [27].
different solutions. Finally, the present method suggests that inhomogeneous spin and charge textures, like stripes or spin polarons, can be viewed as microscopic manifestations of phase separation, as the natural homogeneous solution which can be obtained in mean field has negative compressibility [34].

In conclusion, we show that the half filled stripes observed in experiments in cuprates can be derived using the same methods which lead to the prediction of the existence of (filled) stripes in the Hubbard model [4–7]. The method allows us to describe the quantum transverse fluctuations of the stripes, which are significant (comparable to $t$) for segments of length of 4-6 lattice units. Finally, we present the distribution of $n_{\mathbf{k}}$, with good agreement with experimental results.

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[1] S.-W. Cheong et al, Phys. Rev. Lett. 67, 1791 (1991).
[2] T. E. Mason, G. Aeppli and H. A. Mook, Phys. Rev. Lett. 68, 1414 (1992).
[3] J. Tranquada et al, Nature 375, 561 (1995).
[4] J. Zaanen and O. Gunnarsson, Phys. Rev. B 40, 7391 (1989).
[5] D. Poilblanc and T. M. Rice, Phys. Rev. B 39, 9749 (1989).
[6] H. J. Schulz, Phys. Rev. Lett. 64, 1445 (1990).
[7] A. R. Bishop, F. Guinea, P.S. Lomdahl, E. Louis and J. A. Vergés, Europhys. Lett. 14, 157 (1991); J. A. Vergés, E. Louis, P.S. Lomdahl, F. Guinea and A. R. Bishop, Phys. Rev. B 43, 6099 (1991).
[8] J. A. Vergés, F. Guinea and E. Louis, Phys. Rev. B 46, 3562 (1992).
[9] S. R. White and D. J. Scalapino, Phys. Rev. Lett. 80, 1272 (1998).
[10] M. Fleck, A. I. Lichtenstein, E. Pavarini and A. M. Oleś, Phys. Rev. Lett. 84, 4962 (2000).
[11] C. S. Hellberg and R. Manousakis, Phys. Rev. Lett. 83, 132 (1999).
[12] M. Calandra and S. Sorella, preprint (cond-mat/9911477).
[13] V. J. Emery and S. A. Kivelson, in Proceedings of the First Polish-U.S. Conference on High Temperature Superconductivity (Springer-Verlag, New York, 1996).
[14] S. Caprara et al preprint (cond-mat/9812279).
[15] G. Seibold, E. Sigmund and V. Hizhnyakov, Phys. Rev. B 57, 6937 (1998).
[16] F. Guinea, E. Louis and J. A. Vergés, Phys. Rev. B, 45, 4752 (1992).
[17] E. Louis, G. Chiappe, F. Guinea, J.A. Vergés and E.V. Anda, Phys. Rev. B, 48, 9581 (1993).
[18] E. Louis, F. Guinea, M. P. López-Sancho and J. A. Vergés, Europhys. Lett. 44, 229 (1998). E. Louis, F. Guinea, M. P. López-Sancho and J. A. Vergés, Phys. Rev. B, 59, 14005 (1999).
[19] M. Berciu and S. J ohn, Phys. Rev. B, 61, 10015 (2000).
[20] S. R. White and D. J. Scalapino, Phys. Rev. B 61, 6320 (2000).
[21] S. R. White and D. J. Scalapino, Phys. Rev. Lett. 81, 3227 (1998).
[22] J. Riera and E. Dagotto, Phys. Rev. B 57, 8609 (1998).
[23] G. Fano, F. Ortolani, and A. Parola, Phys. Rev. B 42, 6977 (1990).
[24] G. Gómez-Santos, Phys. Rev. Lett. 70, 3780 (1993).
[25] A. J. Heeger, S. Kivelson, W. P. Su and J. R. Schrieffer, Rev. Mod. Phys. 60, 781 (1988).
[26] M. Bosch, W. van Saarloos and J. Zaanen, preprint (cond-mat/0003239).
[27] X. J. Zhou et al, Science 286, 268 (1999).
[28] A. Castro-Neto and F. Guinea, Phys. Rev. Lett. 80, 4040 (1998).
[29] A. L. Chernyshev, A. H. Castro-Neto and A. R. Bishop, Phys. Rev. Lett. 84, 4922 (2000).
[30] M. Ichikawa and K. Machida J. Phys. Soc. Jpn. 68, 4020 (1999).
[31] M. G. Zacher, R. Eder, A. Arrigoni and W. Hanke, preprint (cond-mat/0005173).
[32] The CI method allows for a systematic inclusion of spin fluctuations, by adding configurations in which the spins along a bond are flipped. We have checked that these configurations do not change qualitatively the results. See also C. Buhler, S. Yunoki and A. Moreo, Phys. Rev. Lett. 84, 2690 (2000).
[33] C. B. Martins et al, Phys. Rev. Lett. 84, 5844 (2000).
[34] F. Guinea, E. Louis, M. P. López-Sancho and J. A. Vergés, Solid State Commun. 113, 593 (2000).