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Spin and charge fluctuations in the U-t-t' model

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As additional neutron scattering experiments are performed on a variety of high temperature superconducting compounds it appears that magnetic incommensuration is a phenomenon common to all of the samples studied. The newest experimental results indicate that incommensurate peaks exist at momentum $\mathbf{q}=\pi(1,1\pm\delta)$ and $\pi(1\pm\delta,1)$ in $La_{2-x}Sr_xCuO_4$ (LSCO) and $YBa_2Cu_3O_{7-\delta}$ (YBCO). The dependence of δ with hole doping appears to be similar in both materials. In addition, new angle-resolved photoemission spectroscopy (ARPES) data for LSCO as a function of doping show that its Fermi surface is qualitatively similar to the one of YBCO, contrary to what was previously believed. Early theoretical attempts to explain the behavior of LSCO and YBCO usually relied on one- or three-band Hubbard models or the t-J model with electron hopping beyond nearest neighbor and with different parameter values for each material. In this paper it is shown that using a one-band Hubbard U-t-t' model with $U/t=6$ and $t'/t\approx-0.25$, good agreement is obtained between computational calculations and *both* neutron scattering and ARPES experiments for LSCO and YBCO. It is also shown that using a more negative t'/t will induce short-range magnetic incommensuration along the diagonal direction in the Brillouin zone, in qualitative disagreement with the experimental results. At the finite temperatures of the present Monte Carlo simulation it is also observed that in this model the tendency to incommensuration appears to be more related to the shape of the two-dimensional Fermi surface and the strength of the interaction, rather than to charge order. [S0163-1829(99)05615-5]

I. INTRODUCTION

Neutron scattering experiments continue providing exciting information about the behavior of spin and charge degrees of freedom in the high T_c cuprates. Studies on $La_{2-x}Sr_xCuO_4$ (LSCO) (Ref. 1) have shown the existence of incommensurability in the spin channel near the commensurate position (π,π). In this case, the incommensurate peaks were found at $Q_\delta=\pi(1\pm\delta,1)$ and $\pi(1,1\pm\delta)$. The value of δ increases linearly with doping in the range $0.05\leqslant x\leqslant 0.14$, while for $x\geqslant 0.14$, δ plateaus at 0.25.[2] The intensity at $Q_\gamma=\pi(1\pm\delta/2,1\pm\delta/2)$ was observed to be 0.18 times that at Q_δ for $x=0.14$ while the intensity at $Q_\pi=(\pi,\pi)$ was negligible compared with the background.[3]

For some time neutron scattering experiments in $YBa_2Cu_3O_{7-\delta}$ (YBCO) were less clear. Rossat-Mignod and co-workers detected magnetic fluctuations only at the commensurate position,[4] while Tranquada *et al.*[5] noticed possible incommensurate fluctuations. Measurements by Dai, Mook, and Dogan,[6] using a new position-sensitive detector bank indicate that incommensurability in the spin channel indeed is present in YBCO. Although originally incommensurability was detected only along the diagonal direction in the Brillouin zone, the latest results indicate that it occurs at Q_δ as in the case of LSCO, and the dependence of δ with doping appears to be similar in both materials.[7]

In addition, $Bi_2Sr_2CaCu_2O_8$ has recently been studied by Mook and Chakoumakos[8] and an incommensurate fluctuation that occurs below T_c was found. This incommensuration was identified with a dynamic charge density wave because its scattering intensity appeared to increase with increasing momentum transfer. Scattering that could be described as magnetic has not been observed yet in this material because the experimental technique used does not allow to reach high enough values of the momentum transfer. However, magnetic excitations should be present if a dynamic strip phase gives origin to the charge peaks. Evidence of incommensurability in the charge channel was also observed in $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$,[9] which led to speculations about a similar behavior in LSCO. This would indicate that the incommensuration in the spin channel may be due to the existence of charge-stripe order rather than to some kind of charge uniform spiral spin state or two-dimensional (2D) Fermi surface effects.[10]

While some of these experiments suggest that magnetic incommensurability in the cuprates may be due to charge-stripe order in which the orientation of the stripes is not material dependent, the theoretical understanding of this phenomenon is less clear. Short-range magnetic incommensurate correlations in the spin channel were detected early on in the Hubbard[11,12] and t-J (Ref. 13) models. The split of the commensurate peak was observed to be qualitatively similar to the behavior in LSCO and YBCO. However, the dependence of δ with doping did not reproduce the experimental data and, as will be shown later, the experimentally observed relative intensities of the peaks at different points in the Brillouin zone are not well reproduced either. No particular order was reported in the charge channel in these models through

numerical analysis.[14,15] However, since the proposal of dynamical phase separation in the CuO_2 planes,[16] a reanalysis of these conclusions is needed.

At the same time that the recent neutron scattering experiments were reporting new similarities between the magnetic properties of the different cuprates, recent angular-resolved photoemission spectroscopy (ARPES) experiments performed on LSCO mapped its Fermi surface[17] (FS) at different values of doping, unveiling interesting similarities among the qualitative FS shape of several high T_c materials.

Motivated by all these new experimental results the aim of this paper is to revisit the U-t-t' model, exploring numerically the spin and charge channels to determine whether it is possible to obtain agreement with the new data for LSCO and YBCO using a unique set of parameters in the model. It will be concluded that this is indeed possible. The paper is organized as follows. In Sec. II the U-t-t' Hamiltonian and the notation used are introduced. Results on magnetic and charge correlations, as well as on the shape of the Fermi surface, are presented in Sec. III while Sec. IV is devoted to the conclusions.

II. THE MODEL

The U-t-t' one-band Hubbard model Hamiltonian is given by

$$H=-t\sum_{\langle \mathbf{ij}\rangle,\sigma}(c^{\dagger}_{\mathbf{i},\sigma}c_{\mathbf{j},\sigma}+\text{H.c.})-t'\sum_{\langle \mathbf{in}\rangle,\sigma}(c^{\dagger}_{\mathbf{i},\sigma}c_{\mathbf{n},\sigma}+\text{H.c.})$$
$$+U\sum_{\mathbf{i}}(n_{\mathbf{i}\uparrow}-1/2)(n_{\mathbf{i}\downarrow}-1/2)+\mu\sum_{\mathbf{i},\sigma}n_{\mathbf{i}\sigma}, \tag{1}$$

where $c^{\dagger}_{\mathbf{i},\sigma}$ creates an electron at site $\mathbf{i}$ with spin projection σ, $n_{\mathbf{i}\sigma}$ is the number operator, the sum $\langle \mathbf{ij}\rangle$ runs over pairs of nearest-neighbor lattice sites, and the sum $\langle \mathbf{in}\rangle$ runs over pairs of lattice sites along the plaquette diagonals. U is the on site Coulombic repulsion, t the nearest-neighbor hopping amplitude, t' the diagonal hopping amplitude, and μ the chemical potential. In this work t will be set equal to 1.

The static charge and magnetic structure factors $N(\mathbf{q})$ and $S(\mathbf{q})$ are defined by the relations

$$N(\mathbf{q})=\sum_{\mathbf{r}}e^{i\mathbf{q}\cdot\mathbf{r}}\langle \delta n_{\mathbf{0}}\delta n_{\mathbf{r}}\rangle, \tag{2}$$

$$S(\mathbf{q})=\sum_{\mathbf{r}}e^{i\mathbf{q}\cdot\mathbf{r}}\langle S^z_{\mathbf{0}}S^z_{\mathbf{r}}\rangle, \tag{3}$$

where $\langle \delta n_{\mathbf{0}}\delta n_{\mathbf{r}}\rangle$ and $\langle S^z_{\mathbf{0}}S^z_{\mathbf{r}}\rangle$ are equal-time density- and spin-correlation functions, $S^z_{\mathbf{r}}=\frac{1}{2}\Sigma_{\alpha,\beta}c^{\dagger}_{\mathbf{r},\alpha}\sigma^z_{\alpha,\beta}c_{\mathbf{r},\beta}$, and $\delta n_{\mathbf{r}}=\Sigma_{\sigma}c^{\dagger}_{\mathbf{r},\sigma}c_{\mathbf{r},\sigma}-\langle n\rangle$. Here $\langle n\rangle=1-x$ is the average density of electrons. The brackets in Eqs. (2) and (3) refer to thermal averaging in the grand canonical ensemble which will be performed using the standard quantum Monte Carlo (QMC) determinantal method.

Before presenting our results let us discuss the behavior of the spin and charge correlations in the noninteracting system ($U/t=0$), and also in the standard Hubbard model with $t'=0$. In the noninteracting system the spin and charge correlations are related through $S(\mathbf{q})=\frac{1}{4}N(\mathbf{q})$. $N(\mathbf{q})$ increases from zero, reaching the value $\langle n\rangle$ at $q=2k_F$ and remaining constant afterwards. On the other hand, in the Hubbard model it was observed that at low density, i.e., $\langle n\rangle<0.5$, $S(\mathbf{q})$ peaks at $q=2k_F$ while $N(\mathbf{q})$ is suppressed at these momenta compared with the noninteracting system and it only peaks at $\mathbf{q}=(\pi,\pi)$.[14] This peak is due to the short-range effective repulsion between particles. The behavior at higher densities is very different in the spin channel. At half filling a sharp peak develops at Q_π and, with a substantially reduced intensity, it moves to Q_δ with doping. While the intensity is maximum at Q_δ as in the experiments, the weight at Q_π is always larger than the one at Q_γ,[11] which is qualitatively incorrect compared with recent experiments, as will be shown below.

III. RESULTS

Due to the well known ''sign problem'' it is very difficult to perform Monte Carlo numerical studies at small hole doping, low temperatures, and values of $U/t>4$. This problem is exacerbated as the absolute value of t' increases. For this reason the numerical efforts will be concentrated here on the study of the fixed density $\langle n\rangle=0.7$ (i.e., $x=0.3$) since for this $\langle n\rangle$ a good degree of control of the numerical results can be achieved. In addition, new experiments have been performed in LSCO at precisely $x=0.3$ providing information about incommensuration[2] and the shape of the FS.[17] Here results for $U/t=6$ on 8×8 lattices will be presented. Due to the sign problem at this relatively large value of U/t, and using a finite diagonal hopping t', the temperature had to be fixed at $T=0.25t$. It is to be expected that the intensity of the observed features will increase at lower temperatures and the results presented here are, thus, lower bounds to the actual values.

The relevant values of $|t'/t|$ range in principle from 0 to 1. However, for values larger than 0.5 the bottom of the band in momentum space moves from (0,0) to $(\pm\pi,0)$ and $(0,\pm\pi)$ in the noninteracting case, qualitatively changing the Fermi surface. Thus, the actual relevant range of values for $|t'/t|$ is between 0 and 0.5.

Note that as part of our study, runs for other values of U/t were performed and qualitative differences with the results for $U/t=6$ were not observed. In particular, for $t'/t=0$ we found that for values of U/t as high as 10 the magnetic incommensuration always occurs at Q_δ rather than along the diagonal as predicted by mean-field calculations in the strong coupling regime.[18]

A. Magnetic incommensurability

As a first step, the static structure factor will be calculated for several values of t'/t and comparisons with the experimental neutron scattering results will be made along several directions in momentum space.

In Fig. 1(a) the peaks in $S(\mathbf{q})$, indicative of short-range spin incommensurate tendencies in the U-t-t' model, are presented along the $(0,\pi)$-$(2\pi,\pi)$ direction for values of t'/t ranging from 0 to -0.5. The figure shows that for all values of t'/t analyzed here, the peak in the structure factor occurs at $\mathbf{q}=(3\pi/4,\pi)$ and $(5\pi/4,\pi)$ which correspond to $\delta=0.25$. This is in agreement with the experimental value

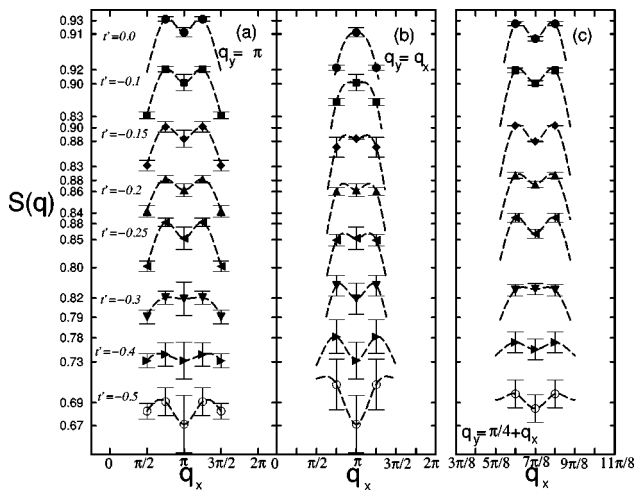

FIG. 1. The static structure factor $S(\mathbf{q})$ for $U/t=6$, $\langle n\rangle=0.7$ on an 8×8 lattice for $T=0.25t$ and values of t'/t ranging from 0 to -0.5. (a) Along the $(\pi,0)$-$(\pi,2\pi)$ direction; (b) along the diagonal direction; (c) along the $q_y=\delta\pi+q_x$ direction. The dashed line indicates a spline fit.

for $x=0.3$ in LSCO.[2] However, a spline fit through the available data points (dashed line) suggests that the actual peak at $|t'/t|\geqslant0.3$ occurs at a slightly larger value of δ. Actually, when the structure factor is scanned along the diagonal direction as shown in Fig. 1(b) it is clear that the results with $|t'/t|=0.3$ or larger do not fit the experimental data because the maxima in $S(\mathbf{q})$ at $\mathbf{q}=(1\pm\delta)\pi(1,1)=(3\pi/4,3\pi/4)$ and $(5\pi/4,5\pi/4)$ have intensities which are approximately equal to or higher than those at Q_δ,[19] as can be deduced by comparing Fig. 1(a) with Fig. 1(b). This is in disagreement with the experiments that indicate that the intensity at $\mathbf{q}=(1\pm\delta)\pi(1,1)$ should be indistinguishable from the background.[2,3,6,7]

An important result is that at $t'=0$ $S(\mathbf{q})$ along the diagonal direction, $\mathbf{q}_x=\mathbf{q}_y$, has a maximum at $\mathbf{q}=Q_\pi$ as can be observed in Fig. 1(b) (top curve). This behavior is in disagreement with the experimental data for LSCO presented in Fig. 3 (closed circles) of Ref. 3, and for YBCO in Fig. 1(c) of Ref. 6 where a minimum is observed at Q_π along the diagonal. The experimental results were obtained at $x=0.15$ for optimally doped LSCO and $x=0.1$ (i.e., $\delta=0.4$) for YBCO showing that the qualitative behavior does not depend strongly on doping. This indicates that the standard Hubbard model ($t'=0$) does not describe the qualitative behavior observed with neutron scattering when $\delta=0.25$. However, working with $t'=-0.2$ the fit along the diagonal in momentum space [Fig. 1(b)] indicates that $S(Q_\pi)$ now has become a local minimum, in qualitative agreement with the experiments. Then, the constraints on the relative intensity of the peaks provided by the experiments leave a finite window of possible values of t'/t. If $|t'/t|\geqslant0.3$ the incommensurate peaks will appear along the diagonal rather than at Q_δ (as discussed in the preceding paragraph) and if $|t'/t|\leqslant0.2$ the structure factor at Q_π would be a local maximum rather than a minimum along the diagonal direction. Note that this window naively seems small, but the effects of $|t'/t|$ on the noninteracting Fermi surface can be shown to be substantial in this range of $|t'/t|$ hoppings. In addition, the effect of $|t'|$ is enhanced by the renormalization of t towards smaller values due to the existence of short-range spin correlations that disfavor same sublattice hopping of holes.

Additional experimental measurements[3] have been reported along the direction $Q_\delta[=\pi(1-\delta,1)]\rightarrow Q_\gamma[=\pi(1-\delta/2,1+\delta/2)]\rightarrow Q_\delta[=\pi(1,1+\delta)]$. Note that for $\delta=0.25$ the point Q_γ is given by $(7\pi/8,9\pi/8)$ which is computationally accessible only on 16×16 or larger lattices if periodic boundary conditions are being used. Since such a large lattice size is beyond the capabilities of the QMC at finite hole density we obtained the values of $S(\mathbf{q})$ at the equivalent Q_γ points located at $7\pi/8(1,1)$ and $9\pi/8(1,1)$ with the help of a spline fit of the available data in Fig. 1(b) (dashed line).

In Fig. 1(c) the structure factor is shown along the line $q_y=\delta\pi+q_x$ which corresponds to the direction along which the experimental neutron scattering data shown by open circles in Fig. 3 of Ref. 3 were taken. In the figure it can be seen that the relative intensity of the numerical data at $q_x=\pi(1-\delta/2)=7\pi/8$, (i.e., Q_γ) and $q_x=\pi(1\pm\delta)=0.75\pi$ or 1.25π (i.e., Q_δ) is a function of t'. Considering, as in the experiments, that the intensity for $\mathbf{q}=\pi(1\pm\delta)(1,1)$ [this point corresponds to $q_x=3\pi/4$ and $5\pi/4$ in Fig. 1(b)] has to correspond to the background, then the relationship $Q_\gamma/Q_\delta=0.18$ is satisfied for $t'/t=-0.25$. This is used as a guide because this relationship may be doping dependent but since the window in t'/t is so narrow, at most an error of the order of 0.05 in the estimation of t'/t is being made.

The above analysis shows that a comparison of the present numerical data when the measured incommensurability δ is 0.25 agrees with the data for LSCO with the same δ using $U/t=6$ and $t'/t=-0.25\pm0.05$. Notice that the position and the relative intensity of the peaks does not change too much with temperature according to the experiment. As in the experiment we also observed that the intensity of the incommensurate peak decreases with the density of electrons.

B. Fermi surface

The next issue to be addressed is highly nontrivial. For the consistency of the results discussed in this paper we must show that the ratio $t'/t=-0.25$, fixed by the spin structure factor analysis in the preceding subsection, will fit other experimental data such as, for example, the shape of the Fermi surface recently obtained using ARPES for LSCO.[17] The possible shape of the FS will be determined by analyzing the momentum distribution $n(\mathbf{q})$ which is calculated by Fourier transforming the one-electron Green function,

$$g_{\mathbf{ij}}=-\left\langle\sum_\sigma c_{\mathbf{i},\sigma}c^\dagger_{\mathbf{j},\sigma}\right\rangle, \tag{4}$$

that is evaluated using QMC.

The criteria used here to obtain the most probable locus of the FS from numerical $n(\mathbf{q})$ data are two: (a) find the values of $\mathbf{q}$ where $n(\mathbf{q})\approx0.5$[11] and (b) find the values of $\mathbf{q}$ where $n(\mathbf{q})$ changes the most rapidly.[20] For the case of $t'/t=-0.25$ we have observed that both methods provide similar results in the regions close to the diagonal direction in the Brillouin zone, but substantial differences were observed close to the $(0,\pi)$ and $(\pi,0)$ points. While criterion (a) indicated a FS closed around (0,0), criterion (b) indicated a FS

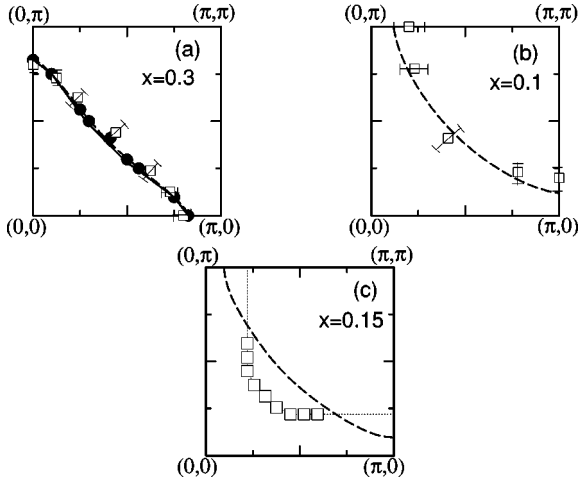

FIG. 2. (a) The numerically calculated Fermi surface for $U/t=6, \langle n\rangle=0.7$ on an 8×8 lattice for $T=0.25t$ and $t'/t=-0.25$ (closed circles and solid line); the open squares are experimental results for LSCO at $x=0.3$ from Ref. 17; the dashed line is the noninteracting, $U/t=0$, FS for $t'/t=-0.25$ and $\langle n\rangle=0.7$; (b) noninteracting ($U/t=0$) FS for $t'/t=-0.25$ and density 0.9 (dashed line) and experimental data for LSCO with $x=0.1$ from Ref. 17; (c) noninteracting FS for $t'/t=-0.25$ and density 0.85 (dashed line) together with experimental data for YBCO with $x\approx0.15$ from Ref. 22.

closed around (π,π). Since criterion (b) provided similar results for the noninteracting case with $\langle n\rangle=0.7$ and $t'/t=-0.25$, a situation where it is known that the FS actually closes around (0,0), it was decided that criterion (a) would be more effective in this context.

The FS obtained with procedure (a) is shown in Fig. 2(a). The closed circles indicate where $n(\mathbf{q})\approx0.5$ and the continuous line is a sixth order polynomial fit of the points. The obtained FS is very similar to the noninteracting one (denoted by a dashed line in the same figure). It satisfies Luttinger's theorem within error bars and, actually it is in excellent agreement with the experimental data for $x=0.3$ (Ref. 17) shown with open squares in Fig. 2(a). Thus, using $t'/t=-0.25$ good agreement has been obtained between the numerical results and two independent experiments (neutron scattering and ARPES) performed in overdoped LSCO. Since the obtained Fermi surface closely resembles the noninteracting one, the FS in the $U/t=0$ limit was calculated for $x=0.1$ and its shape compared directly with the experimental results at this density. As can be observed in Fig. 2(b) the agreement is once again very good. According to Ref. 17 the FS for LSCO at optimal doping is still centered about (π,π) and it is qualitatively similar to the one obtained for $x=0.1$. This is indeed what happens with the $U/t=0$ FS for $t'/t=-0.25$ at $x=0.15$ which is shown in Fig. 2(c) (dashed line). At the noninteracting level the change between a FS that closes around (π,π) and around (0,0) occurs at $x=0.22$ for the ratio of t'/t used here.

In addition, in Fig. 2(c) the experimental points for optimal doped YBCO obtained several years ago[22] are also shown. The agreement with our result is only qualitative but it has to be considered that the measurements are very difficult due to surface effects and thus the experimental points have large error bars (not shown). It is important to remark

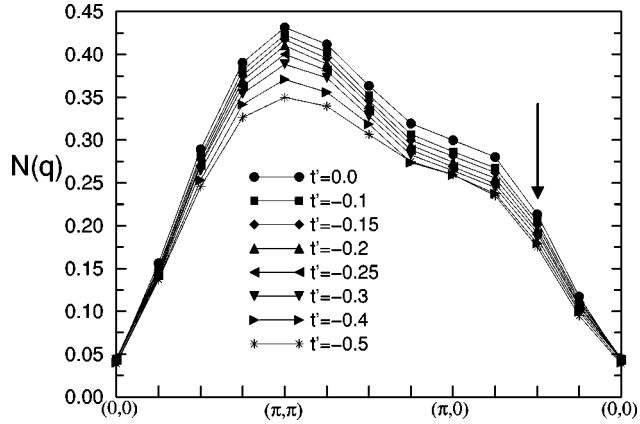

FIG. 3. Static charge structure factor for $U/t=6$, $\langle n\rangle=0.7$ on an 8×8 lattice for $T=0.25t$ and values of t'/t ranging from 0 (top) to -0.5 (bottom) along the directions (0,0)-(π,π)-$(\pi,0)$-(0,0). The arrow indicates the value of the momentum where a maximum indicating incommensurate short-range order would be expected.

that the similarity found between the interacting and the noninteracting FS for $t'/t=-0.25$ does not mean that they are identical, but the differences will be apparent only when larger lattices at lower temperatures can be studied.

In previous literature the experimental results have been interpreted as indicating that there is a FS only along the diagonal direction and no FS close to $(0,\pi)$ and $(\pi,0)$.[21] The rate of change of $n(\mathbf{q})$ could support this view but we found out that it also gets very reduced close to $(0,\pi)$ and $(\pi,0)$ even in the noninteracting case when it is known that there is a continuous FS. Thus, the present results do not allow us to decide one way or the other. We also noticed that the interacting FS for $t'/t=-0.3$ appears to be qualitatively different from the noninteracting one. In particular, at $x=0.3$ it seems to close around (π,π) while the noninteracting one closes around (0,0). Thus, assuming that YBCO has the same qualitative shape of FS than LSCO in the overdoped regime, this provides another reason to rule out values of $|t'/t|$ equal to or higher than 0.3.

C. Charge correlations

The next issue that will be addressed is the origin of the incommensurate magnetic fluctuations in the present model. In Fig. 3 the charge structure factor $N(\mathbf{q})$ along the (0,0) $\rightarrow(\pi,\pi)\rightarrow(\pi,0)\rightarrow(0,0)$ directions for t'/t ranging from 0 (top) to -0.5 (bottom) is shown. In all cases there is a broad maximum at Q_π which is due, as in the low electron density limit of the Hubbard model, to the short-range effective repulsion between particles. If the incommensurate magnetic fluctuations were due to dynamical charge fluctuations, peaks at $\mathbf{q}=\pi(0,2\delta)$ and $\pi(2\delta,0)$ should be observed in $N(\mathbf{q})$ according to previous theoretical studies.[9,16] In the present case, since $\delta=0.25$, the peaks would be expected at $(0,\pi/2)$ and $(\pi/2,0)$. This momentum is indicated with an arrow in Fig. 3 and it is clear from the figure that no indications of incommensurate charge order are observed. It could be argued that charge incommensuration is not observed due to the high temperature in our calculations. However, this

would be an indication that the threshold of temperature for the observation of spin and charge incommensurability is not the same.

Another possible origin of the magnetic incommensuration in 2D could be simple FS effects.[10,23,24] There are some momenta that map points (or regions) of the FS into other points (or regions) also on the FS. These are called nesting or pseudonesting vectors and they correspond to values of momentum where maxima occur in the imaginary part of the magnetic susceptibility in the 2D noninteracting system. We performed a numerical calculation of the pseudonesting vector for the interacting FS. We constructed a histogram in order to identify the value of the momentum that mapped most points of the FS into other points also belonging to it. For $t'/t=-0.25$ at $x=0.3$ a maximum in the histogram was obtained at $\mathbf{q}=(\pi,0.67\pi)$ which is in very good agreement with the analytical value for the corresponding noninteracting FS, namely, $\mathbf{q}=(\pi,0.71\pi)$.[23] Thus, the maximum in $S(\mathbf{q})$ at $\mathbf{q}=(\pi,0.75\pi)$ could be explained by FS effects in this case but it may be due to the coarse grid that necessarily had to be used in our computational studies. In the noninteracting case it is expected that the maximum remains at Q_π until x reaches 0.22 (see Sec. III B). Though this behavior seems to be in agreement with previous results for the interacting case[20] and in disagreement with the experimental data, it is possible that the effect of the interaction at smaller dopings will be observed at lower temperatures than the ones that can presently be reached.

IV. CONCLUSIONS

In summary, motivated by recent neutron scattering and ARPES experiments, we have studied the U-t-t' model numerically on 8×8 lattices at temperature $T=0.25t$ and with coupling $U/t=6$. Fixing the density at $\langle n\rangle=0.7$ agreement between the position and the relative intensity of the incommensurate peaks obtained numerically and experimentally for LSCO and YBCO is observed for $t'/t=-0.25\pm0.05$ which corresponds to a window of 20% within the possible values of $|t'/t|$ that run from 0 to 0.5. Larger values of $|t'/t|$ are ruled out because in this case the structure factor has a maximum along the diagonal direction rather than at Q_δ, while with less negative values of t'/t a relative maximum is observed at Q_π along the diagonal direction, again in disagreement with experimental results. It is possible that for slightly larger values of U/t, such as 8 or 10, the window in $|t'/t|$ that reproduces the experiments may change but by simple continuity it is not expected that these potential changes will be large. Thus, the Hubbard or t-J models without nearest-neighbor electron hopping do not appropriately reproduce this experimental behavior in the cuprates.

The incommensurate magnetic peaks do not seem related to incommensurate charge fluctuations. In the overdoped regime FS effects enhanced by the electronic interactions may be responsible for the observed results. The sign problem prevented the exploration of this issue in the optimal doped and underdoped regimes.

The most exciting result of our paper is that the addition of a diagonal hopping $t'/t=-0.25$ also provides good agreement with experimental angle-resolved photoemission measurements of the FS for LSCO and YBCO at different densities. A FS that closes around (π,π) in the underdoped and optimal doped regimes, and around (0,0) in the overdoped case is observed.

Thus, the present numerical analysis provides good agreement between a theoretical model and two unrelated experiments in the overdoped regime of LSCO. It also shows that the consideration of a diagonal hopping in models for the cuprates is crucial in order to reproduce experimental data. Note that this conclusion is in excellent agreement with ARPES calculations that have focused on the insulating compound $Sr_2CuO_2Cl_2$.[25] For the cases analyzed here, the same ratio t'/t can reproduce results for both LSCO and YBCO. Then, the difference in parameters between LSCO and YBCO observed in previous calculations[26] may need reexamination. Note that the addition of t'' terms may further improve the theory-experiment agreement reported here.[27] Although the behavior of the incommensurate magnetic peaks in the cuprates appear to be similar, there is still no experimental information about relative intensities of the peaks at different points in the Brillouin zone carried out at the same density. These measurements could indicate possible material dependent properties that could be caused by longer-range electron hopping terms.[25]

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