On the contrasting spin dynamics of $La_{2-x}Sr_xCuO_4$, $Nd_{2-x}Ce_xCuO_4$ and $YBa_2Cu_3O_{6+x}$ near half filling

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Abstract

We present simple calculations which show that the incommensurability upon doping and the width of the magnetically ordered phase in Mott-Hubbard insulators depend strongly on the location of the hole/electron pockets in the Brillouin zone. For $LaSrCuO$ systems, we found the pockets at $(\pm \pi/2, \pm \pi/2)$, in which case the corrections to the antiferromagnetic spin stiffness rapidly grow with doping and destroy commensurate spin ordering already at a very small doping. On the other hand, in $NdCeCuO$, the hole pockets are located at $(\pi,0)$ and the symmetry related points, in which case the corrections to the stiffness scale linearly with the density of carriers and do not destroy commensurate spin ordering. For $YBCO$ systems, the situation is less certain, but our results favor hole pockets at $(\pi/2, \pi/2)$. We also briefly discuss the tendency towards phase separation.
I. INTRODUCTION

The intense interest in understanding the properties of high temperature superconductors initiated theoretical research on the behavior of antiferromagnetic insulators upon doping. The parent compounds of high-$T_c$ materials are well described as Heisenberg antiferromagnets. Upon hole doping, long-range antiferromagnetism rapidly disappears and the systems eventually become metallic superconductors. The same transformation occurs in electron-doped materials but at substantially larger doping concentrations. The behavior of the antiferromagnetic insulator upon doping attracted a lot of interest over the past few years as the exchange of antiferromagnetic paramagnons is at least one of the relevant pairing interactions between holes. There are several fundamental issues related to doped antiferromagnets, one of which is whether magnetic correlations remain peaked at $Q_0 = (\pi, \pi)$ upon doping, or shift to incommensurate momenta. Shraiman and Siggia first pointed out that if the dispersion of vacancies has a minimum at $(\pm \pi/2, \pm \pi/2)$, then the dopants introduced into commensurate nearest-neighbor antiferromagnet give rise to a long-range dipolar distortion of the staggered magnetization which may lead to a spiral spin configuration.

It has been recently argued that the values of hopping integrals in electron-and hole doped 214 materials are nearly the same; $t \sim 0.4eV$, $t' \sim -0.2t$, where $t'$ is the nearest-neighbor hopping. Despite this, the incommensurability upon doping has been found only in $LaSrCuO$ compounds while the dynamical structure factor in the doped $NdCeCuO$ remains peaked at $(\pi, \pi)$. Moreover, experimentally, long-range magnetic order in $LaSrCuO$, disappears already at $3-4\%$ doping, while in $NdCeCuO$ it survives up to $12\%$ doping.

The goal of the present paper is to show that the contrasting magnetic dynamics in the two 214 systems near half filling is related to a different location of the hole pockets. Namely, we will argue that in $La$-based materials, the pockets are located at $(\pm \pi/2, \pm \pi/2)$ while in $Nd$- based materials doped electrons occupy pockets centered around $(0, \pm \pi)$ and $(\pm \pi, 0)$. This, as we show below, gives rise to a completely different spin dynamics in the
two materials: the commensurate \((\pi, \pi)\) state rapidly becomes unstable in \(LaSrCuO\), but survives in \(NdCeCuO\).

We will also discuss the location of the hole pockets in \(YBa_2Cu_3O_{6+x}\) where the next-nearest neighbor hopping amplitude is relatively large, \(t' \sim -0.5t\). Our results for the Hubbard model, show that for \(t'/t \sim -0.5\) and \(J/t \sim 0.4\), the mean-field hole dispersion is nearly degenerate along \(k_x = k_y\) and has a flat minimum at \((\pi, \pi)\). However, self-energy corrections still favor pockets at \((\pi/2, \pi/2)\) and are likely to overshadow the small difference between the mean-field quasiparticle energies at \((\pi/2, \pi/2)\) and \((\pi, \pi)\). In this situation, the spin dynamics of \(LaSrCuO\) and \(YBaCuO\) near half-filling are nearly identical, and differ only in the metallic phase where the Fermi surface is large, and in case of \(YBaCuO\), is centered at \((\pi, \pi)\). Notice, however, that cluster calculations for the \(t - t' - J\) model reported hole pockets at \((\pi, \pi)\) for the same ratios of parameters \([5,11]\). If it is actually the case for \(YBaCuO\), the spin dynamics right near half-filling will be very similar to that in the electron-doped materials (see below).

The bulk of our consideration is presented in the next section. We will first briefly review the spin-density wave theory for the Hubbard model near half-filling, then will find the location of the hole pockets for the hole- and electron-doped materials, and next show how the different location of the hole pockets give rise to a contrasting magnetic behavior near half-filling. Finally, we discuss the tendency towards domain wall formation upon doping. Our conclusions are presented in Sec.III.

II. HUBBARD MODEL WITH NEXT-NEAREST-NEIGHBOR HOPPING

We consider the one-band Hubbard model given by

\[
H = -t \sum_{<i,j>} a_{i,s}^\dagger a_{j,s} - t' \sum_{<i,j'>} a_{i,s}^\dagger a_{j',s} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}
\]

Here \(j\) and \(j'\) label the nearest and the next-nearest neighbors, respectively, and \(n = c^\dagger c\) is the particle density. We will use the spin-density-wave formalism \([12]\) which, as has been
shown in a number of papers [12–18], is a good starting point for the calculations close to half-filling. Below we mostly restrict with the simplest mean-field calculations. This last restriction can be formally justified if one extends the Hubbard model to a large number of orbitals at a given site, \( n_c = 2S \), [19] and restrict with the leading term in \( 1/S \) expansion. This mean-field theory is meaningless for the nearest-neighbor Hubbard model because of the accidental degeneracy in the hole spectrum which is lifted only by \( 1/S \) corrections (see the discussion below). However, the nonzero \( t' \) eliminates the accidental degeneracy already at the mean-field level. In this situation, we expect that the corrections to the mean-field results renormalize the parameters of the model, which will be important for our analysis of \( YBaCuO \), but do not give rise to any new physics of the insulating phase.

A. SDW theory at half-filling

We now briefly discuss the key points of the SDW formalism at half-filling. This formalism has been applied several times to the \( t' = 0 \) model. First, we assume that at half-filling, the 2D Hubbard model has a commensurate antiferromagnetic ground state. This implies that, e.g., \( z \) component of the spin-density operator, \( \vec{S}(q) = (1/2) \sum_k a_{k+q,\alpha}^\dagger \vec{\sigma}_{\alpha,\beta} a_{k,\beta} \), has a nonzero expectation value at \( q = Q_0 \). We then use the relation \( \langle \sum_k a_{k+Q,\uparrow}^\dagger a_{k,\uparrow} \rangle = -\langle \sum_k a_{k+Q,\downarrow}^\dagger a_{k,\downarrow} \rangle = \langle S_z \rangle \), to decouple the quartic term in (1). After decoupling, the quadratic Hamiltonian takes the following form

\[
\mathcal{H}_{MF} = \sum_k \epsilon_k^+ (a_{k\sigma}^\dagger a_{k\sigma} + a_{k+Q_0\sigma}^\dagger a_{k+Q_0\sigma}) + \\
\sum_k \epsilon_k^- (a_{k\sigma}^\dagger a_{k\sigma} - a_{k+Q_0\sigma}^\dagger a_{k+Q_0\sigma}) - \\
\sum_k \Delta \text{sgn}(\sigma) (a_{k\sigma}^\dagger a_{k+Q_0\sigma} + a_{k+Q_0\sigma}^\dagger a_{k\sigma})
\]

Primes to the summation signs indicate that the summation is over the reduced Brillouin zone. We introduced \( \Delta = U \langle S_z \rangle \), \( \epsilon_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y \), \( \epsilon^+ = (\epsilon_k + \epsilon_{k+Q_0})/2 = -4t' \cos k_x \cos k_y \), \( \epsilon^- = (\epsilon_k - \epsilon_{k+Q_0})/2 = -2t(\cos k_x + \cos k_y) \). The next step is the diagonalization of the quadratic form by a Bogolyubov transformation.
\[ a_{k,\sigma} = u_k c_{k\sigma} + v_k d_{k\sigma} \]
\[ a_{k+Q_0,\sigma} = \text{sgn}(\sigma)(u_k d_{k\sigma} - v_k c_{k\sigma}) \] (3)

Applying this transformation to (2), we observe that the first term with the density of quasiparticles, indeed, does not depend on \( u_k \) and \( v_k \), because the transformation conserves the total density. The Bogolyubov coefficients then appear only in the last two terms which do not depend on \( t' \). As a result, the expressions for \( u_k \) and \( v_k \) remain the same as in the \( t' = 0 \) model [12]:
\[ u_k = \left[ \frac{1}{2} \left( 1 + \frac{\epsilon_k}{E_k} \right) \right]^{\frac{1}{2}} ; \quad v_k = \left[ \frac{1}{2} \left( 1 - \frac{\epsilon_k^-}{E_k^-} \right) \right]^{\frac{1}{2}} \] (4)

where \( E_k^- = \sqrt{\Delta^2 + (\epsilon_k^-)^2} \).

After the diagonalization, Eq. (2) takes the form
\[ \mathcal{H}_{MF} = \sum_k E_k^- c_{k\sigma}^\dagger c_{k\sigma} - E_k^\dagger d_{k\sigma}^\dagger d_{k\sigma} \] (5)

where
\[ E^c = E_k^- + \epsilon_k^+ , \quad E^d = E_k^- - \epsilon_k^+ \] (6)

For \( U \gg t \), which is implicit in our approach, we can expand under the square root and obtain \( E^{c,d} = \Delta + J(\cos k_x + \cos k_y)^2 \mp 4t' \cos k_x \cos k_y \), where \( J = 4t^2/U \). We will refer to the quasiparticles described by \( c \) and \( d \) operators as conduction and valence fermions, respectively. At half-filling, valence states are occupied and conduction states are empty. Accordingly, the self-consistency condition on \( \langle S_z \rangle \) takes a simple form
\[ \frac{1}{U} = \sum_k ' \frac{1}{E_k^-} \] (7)
At large \( U \), we obtain, as usual, \( \Delta = U/2 \), or \( \langle S_z \rangle \approx 1/2 \).

**B. Finite density of holes**

We now discuss what happens at small but finite doping when the chemical potential moves into the valence band. First, we discuss the shape of the hole Fermi surface. As we said
above, at \( t' = 0 \), the dispersion of valence fermions, Eq.(3), is degenerate along the boundary of the magnetic Brillouin zone \( (k_x \pm k_y = \pm \pi) \), where \( E^d = \Delta \). This degeneracy, however, is not related to any kind of symmetry and is removed by self-energy corrections \([15,17]\), with the result that the actual band minima in the nearest-neighbor Hubbard model are at \((\pm \pi/2, \pm \pi/2)\). This agrees with the numerical \([24,20,25]\) and variational \([26]\) studies of the Hubbard and \( t-J \) models.

Our first observation for \( t-t'-U \) model is that at finite \( t' \), the degeneracy is removed at the mean-field level. Indeed, a simple inspection of Eq.(8) shows that the mean-field dispersion has a minimum at \((\pm \pi/2, \pm \pi/2)\) if \( t' \) is negative and smaller than \( J \). For \( |t'| > J \), the minimum of the hole dispersion is at \( k = (\pi, \pi) \) (or \((0, 0)\)). Finally, if \( t' \) is positive, which is probably not the case for cuprates, the minimum of \( E^d \) is at \((\pi, 0)\) and symmetry related points \([24]\). Now, for both 214 compounds, \( t' \) is negative and relatively small: \( |t'| \sim 0.07ev \), which is smaller than the exchange integral \( J \sim 0.13ev \) \([21,23]\). Accordingly, we expect that upon doping, holes in \( La- \) based compounds form pockets around \((\pi/2, \pi/2)\) and the symmetry related points. Near \((\pi/2, \pi/2)\), one can expand \( E^d_k \) and obtain

\[
E^d_k = \Delta + \frac{k^2_{\perp}}{2m_{\perp}} + \frac{k^2_{\parallel}}{2m_{\parallel}}
\]  

(8)

where \( m_{\perp} = 1/4(J - |t'|) \), \( m_{\parallel} = 1/4|t'| \). Notice that numerically, the effects due to \( t' \), even for \( |t'|/t | \sim 0.2 \) are likely to dominate over the effects due to self-energy corrections in nearest-neighbor model. Thus, for \( t/J = 2 \), the difference \( \Delta E = E^d(\pi, 0) - E^d(\pi/2, \pi/2) \) is \( \Delta E = 4|t'| \sim 0.8t \) due to \( t' \) and about 0.25\( t \) due to quantum fluctuations as was obtained in \( 1/S \) expansion for the Hubbard model \([17]\) and in numerical \([25]\) and variational \([20]\) calculations for the \( t-J \) model. The same is also true for the inverse effective mass, \( 1/m_{\parallel} \): for the same ratio \( t/J \), the contribution to \( 1/m_{\parallel} \) due to \( t' \) is about four times larger than due to quantum fluctuations. Also notice that for the parameters chosen for \( LaSrCuO \), the two effective masses are roughly equal to each other, i.e., the Fermi surface near half-filling is nearly circular.

Consider now the electron-doped materials. Under the electron doping, the chemical
potential moves into the conduction band. The energy of a conduction fermion is $E^c = \Delta + J(\cos k_x + \cos k_y)^2 - 4t' \cos k_x \cos k_y$, i.e. it effectively has the sign of $t'$ reversed compared to the hole-doped materials. From the consideration above, we immediately conclude that the minimum of the electron dispersion is at $(0, \pi)$ and the symmetry related points. The same is, indeed, true also for the selection due to quantum fluctuations in the nearest-neighbor model. Expansion around the minima yields two equivalent effective masses $m_\perp = m_\parallel = 1/4|t'|$.

Finally, consider the electron dispersion in the $Y-$ based hole-doped materials. The spin dynamics of the overdoped 123 systems was studied in a number of papers by K. Levin, Q. Si and coauthors [9]. They found that to fit the photoemission data for $YBa_2Cu_3O_7$ [8], one needs $t \sim 0.25-0.3ev$ and relatively large next-nearest-neighbor hopping term $t' \sim -0.5t$ [9]. The values of the hopping integrals right near half-filling are not necessary the same as in $YBa_2Cu_3O_7$ as the parameters of the effective one-band Hubbard model derived from the underlying three-band model generally depend on doping [27]. We however simply assume that the values of $t$ and $t'$ change little with decreasing oxygen content. In this situation, $|t'|$ is very close to $J$. This implies that the mean-field hole dispersion, Eq(3), is nearly degenerate along $k_x = k_y$: the band minima at $t = 0.3ev$ is at $(\pi, \pi)$, but the quasiparticle energy at $(\pi/2, \pi/2)$ is only $0.08ev$ above. To lift the near degeneracy, we calculated the leading self-energy correction to the hole dispersion in the expansion over the inverse number of orbitals. The procedure is described in some length in our earlier publication [17], and we do not discuss it here. We found, that fluctuations stabilize the minima at $(\pm \pi/2, \pm \pi/2)$ up to much larger $t'$ than in the mean-field theory. Specifically, the self-energy terms produce the energy difference, $\Delta E \sim 0.88\Delta$ (for $2S' = 1$), where $\Delta E = E_{(\pi,\pi)} - E_{(\pi/2,\pi/2)}$. For $t = 0.3ev$, we have $\Delta = 4t^2 < S_z > /J \sim 0.9ev$ [28] and hence $\Delta E \sim 0.8ev$. This implies that the actual critical value of $|t'|$ above which pockets are located at $(\pi, \pi)$, is about $0.32ev$, which is substantially larger than $|t'| \sim 0.13 - 0.15ev$ predicted for $YBaCuO$.

The hole pockets at $(\pm \pi/2, \pm \pi/2)$ near half-filling are consistent with the results of photoemission studies of the insulating $YBa_2Cu_3O_{6.3}$ [29]. These studies have detected some spectral features which can be interpreted as the dispersion through Fermi surface,
but only close to the zone diagonal, i.e., near \((\pi/2, \pi/2)\). Notice however that the closed Fermi surface near that point has not been restored experimentally.

Another important point is that the critical value of \(t'\) is indeed model dependent - in the Hubbard-model calculations we found that it is larger than in \(YBaCuO\), but, as we already mentioned in the Introduction, small cluster calculations for the \(t-t'-J\) model found the minimum of hole dispersion at \((\pi, \pi)\) for the same values of parameters as we used \[5\].

We further show how the different location of the pockets leads to a contrasting magnetic behavior near half-filling.

C. Magnetic susceptibility

In the SDW theory, the spin susceptibility is given by a ladder series of bubble diagrams (Fig.1). One fermion in the bubble should be above the Fermi surface, and one below. At half-filling, the only allowed combination is one fermion from the conduction and one the from valence band. Away from half-filling, the Fermi level moves into the valence band, and there are also bubbles with two valence fermions. The SDW expression for the susceptibility has been derived earlier \[12,16\], so we quote only the result. In the static case, the total transverse susceptibility \(\chi^{+-}(q)\) is given by

\[
\chi^{+-}(q) = \frac{\chi_0(q)}{1 - U\chi_0(q)}
\]  

where

\[
\chi_0^{+-}(q) = \frac{1}{2N} \sum_{E_d > |\mu|} \left[ 1 - \frac{\epsilon_k \epsilon_{k+q} - \Delta^2}{E_k E_{k+q}} \right] \left( \frac{1}{E_k + E_{k+q}} + \frac{1}{E_d + E_{k+q}} \right)
\]

\[
\frac{1}{N} \sum_{E_d > |\mu| \atop E_d < |\mu|} \left[ 1 + \frac{\epsilon_k \epsilon_{k+q} - \Delta^2}{E_k E_{k+q}} \right] \frac{1}{E_{k+q} - E_k}
\]

Above we assumed that the system has a commensurate magnetic order. This requires that the static spin susceptibility be non-negative for all momenta (or, in other words, that all bosonic frequencies be real). Of special interest is the region near \(q = Q_0 = (\pi, \pi)\) as
\( \chi^{-1}(q) \) turns to zero at \((\pi, \pi)\) in accordance with the Goldstone theorem. Near this point, the static susceptibility has the form \([30]\)

\[
\chi^{+-}(q) = \frac{2N_0^2}{\rho_s(q - Q_0)^2}
\]  

(11)

where \(N_0\) is sublattice magnetization \((= 1/2\) in our mean-field approach), and \(\rho_s\) is the spin stiffness which should be positive.

Let us first consider half-filling. Here only the first term contributes to \(\chi_0\). Performing an expansion in (10) and substituting the result into (9), we obtain the “classical” spin wave result

\[
\rho_s = \frac{1}{4} J \left( 1 - \frac{2(t')^2}{t^2} \right)
\]

(12)

Clearly then, the commensurate \((\pi, \pi)\) state is stable at half-filling as long as \(\sqrt{2}|t'| < t\). This condition, though it may be modified by quantum fluctuations, is apparently satisfied in the \(LaSrCuO\), \(NdCeCuO\) and \(YBaCuO\) families.

We further consider the situation away from half-filling \((\delta \neq 0)\). Now we also have a contribution from the second term which involves only valence fermions. Expanding in this term around \((\pi, \pi)\) and combining the result with (12), we obtain

\[
\rho_s(\delta) = \rho_s(0) \left( 1 - \frac{\rho_s(\delta)}{\rho_s(0)} \right)
\]

(13)

where \(\rho_s(\delta = 0)\) is given by (12), and \(z\) is

\[
z = 4U \frac{1}{N} \lim_{q \to 0} \sum_{E_k^d < |\mu|} \frac{\sin^2 k_x}{E_{k+q}^d - E_k^d}
\]

(14)

At small concentration of holes, the condition \(E_{k}^d < |\mu|\) implies that the fermion with momentum \(k\) is within the hole pocket. For \(La\) and \(Y\)-based materials, these pockets are at \((\pm \pi/2, \pm \pi/2)\) where the \(\sin^2 k\) factor in the numerator in (14) is approximately one. Accordingly, the summation over \(k\) yields the uniform Pauli susceptibility of free fermions, which in two spatial dimensions does not depend on the carrier concentration. Namely, for \(z\) we obtain
\[
 z = 2U_{\text{eff}} \frac{\sqrt{m_\perp m_\parallel}}{\pi} 
\]

For the case of \((\pi/2, \pi/2)\) pockets, \(|t'| \leq J\), so that \(\sqrt{m_\perp m_\parallel}\) scales as \(1/J\). In the mean-field theory, we also have \(U_{\text{eff}} = U\) in which case \(z \sim U/J\) is a large number, and the spin stiffness immediately changes sign upon doping which means that the commensurate \((\pi, \pi)\) antiferromagnetic state becomes unstable. In more sophisticated calculations however, \(U_{\text{eff}}\) appears different from \(U\) because of the strong self-energy and vertex corrections in the large-\(U\) limit. In fact, the self-consistent solution for \(U_{\text{eff}}\) yields \(U_{\text{eff}} \sim J\) at \(U \gg t\), and therefore \(z \sim O(1)\) \[2,31,16\]. Moreover, extremely close to half-filling, \(z\) vanishes logarithmically as \(z \sim 1/|\log \delta|\) because of the logarithmical singularity in the 2D scattering amplitude \[16\].

In any event, however, \(z\) rapidly grows with doping, and it is very likely that it quickly becomes larger than one in which case the commensurate antiferromagnetic state is no longer stable. Note that in the mean-field approach we are using, this instability does not imply a disordering transition, but rather a transformation into an incommensurate spin configuration. The equilibrium configuration at \(z > 1\) has been discussed in our separate publication \[18\].

We now turn to the electron-doped systems. Here the hole pockets are formed around \((0, \pi)\). Eq.\((13)\) and \((14)\) are still valid, but the numerator in \((14)\) now vanishes right at the center of the pocket. Elementary calculations then show that because of the \(\sin^2 k\) factor in \((14)\), \(z\) scales linearly with doping concentration, and hence at small doping, \(\rho_s\) acquires only a small correction \(O(\delta)\). Clearly then, antiferromagnetism at \((\pi, \pi)\) survives in the presence of a small density of electrons. This explains why \(Nd_{2-x}Ce_xCuO_4\) remains commensurate all the way down to the paramagnetic phase.

We now discuss the width of the magnetically ordered phase. Within the present mean-field (or large \(S\)) approach, the on-site magnetization is nearly equal to its nominal value, and the rapid decrease in the stiffness in the hole doped 214 materials is not accompanied by the rapid decrease in the order parameter. In other words, the mean-field theory predicts that the system first becomes incommensurate and only then loses long-range order. There
are, however, numerous experimental reasons to believe that the disordered transitions in weakly doped high-$T_c$ materials are in the universality class of the nonlinear sigma model with the dynamical exponent $\tilde{z} = 1$ \[32\] (the most direct evidence is the observed linear behavior of the uniform susceptibility). This implies than in a more adequate model, the decrease in $\rho_s$ must eventually lead to the decrease in the sublattice magnetization such that both quantities vanish simultaneously. This is what has been found by Sachdev \[33\] in the self-consistent large-N study of the Shraiman-Siggia model \[2\] in some range of the coupling constant values. In another range, he found an incommensurate transition within the ordered phase like in our approach. It is essential however, that the two scenarios differ primarily in the behavior of the sublattice magnetization with doping, while the doping dependence of the spin stiffness is nearly the same in both cases. In particular, for all values of the coupling constant in the Shraiman-Siggia model (where pockets are at $(\pi/2, \pi/2)$), the stiffness undergoes a rapid, nearly step-like, downturn renormalization under hole doping. We can, therefore, expect that the larger are the corrections to the stiffness at low doping (even if they are obtained in large-$S$ expansion, as in our approach) the smaller is the actual region of the magnetically ordered phase. Thus the width of the magnetically ordered phase in $NdCeCuO$ should be much larger than in $LaSrCuO$. This is consistent with the experimental observation that magnetic order in $NdCeCuO$ survives up to much larger doping concentrations than in $LaSrCuO$. A similar, though somewhat different, explanation of the difference of the magnetic phase diagrams of the two 214 compounds, based on the idea of localized electrons in $NdCeCuO$ and mobile holes in $LaSrCuO$, was presented in \[3\].

Finally, we notice that if the actual ratio of $t'/t$ is such that the pockets in $YBaCuO$ at low doping are located at $(\pi, \pi)$, then the corrections to the stiffness scale linearly with $x$ by exactly the same reasons as in the electron-doped compounds, and the commensurate $(\pi, \pi)$ configuration survives the hole doping.
D. Phase separation

In SDW approach, we can also consider stability of the \((\pi, \pi)\) phase at small doping against the formation of domain walls \[34,35\]. This stability requires the longitudinal spin susceptibility to be positive. For the commensurate spin ordering, longitudinal spin fluctuations are always decoupled from transverse spin fluctuations, but at finite doping, they are coupled to charge fluctuations. The total static uniform susceptibility \(\chi^{zz}\) can be obtained by straightforward manipulations starting from Eq.(52)-(54) in \[16\]:

\[
\chi^{zz} \approx \frac{2\chi^{\text{Pauli}}}{1 - 8J\chi^{\text{Pauli}}}
\]

where \(\chi^{\text{Pauli}} = \sqrt{m_{\perp}m_{\parallel}}/2\pi\) is the Pauli-like susceptibility of doped carriers. If this susceptibility is larger than \(1/8J\), the total longitudinal susceptibility becomes negative which signals the formation of domain walls.

We calculated effective masses with self-energy corrections for all three types of materials, and found that for \(|t'| \sim J/2\), the tendency towards phase separation is nearly the same in the two 214 compounds (the Pauli susceptibility is slightly larger in \(LaSrCuO\)), and is much weaker in \(YBaCuO\) where the Pauli susceptibility is about two times smaller. At the same time, we found that the denominator in \(\chi^{zz}\) is positive in 214 materials, i.e., there is a stability against domain wall formation immediately away from half-filling. These results are consistent with the numerical analysis in Ref. \[3\]. The latter paper also points to a possibility of a two-dimensional phase separation in the electron-doped materials which we didn’t study.

III. CONCLUSIONS

To summarize, in this paper we presented simple calculations which show that the stability of the commensurate antiferromagnetic state in the Mott-Hubbard insulators depends strongly on the location of the hole/electron pockets in the Brillouin zone. For \(LaSrCuO\), we found pockets at \((\pm \pi/2, \pm \pi/2)\). The corrections to the antiferromagnetic spin stiffness from
the occupied hole states within these pockets rapidly grow with the carrier concentration and are likely to make stiffness negative, i.e., destroy commensurate spin ordering, already at a very small doping. On the other hand, in $NdCeCuO$, we found that mobile electrons form pockets at $(0, \pi)$ and the symmetry related points, in which case the corrections to the stiffness scale linearly with the density of carriers and do not destroy the commensurate spin ordering. We argued that the different behavior of stiffnesses is responsible for the experimentally observed difference in the widths of the magnetically ordered phases in the two 214 compounds. These results compliment the arguments and numerical analysis in Ref [5].

We also discussed the hole dispersion in $YBaCuO$ and found that for the value of $t'$ used to fit the photoemission data, band minima are likely to remain at $(\pm \pi/2, \pm \pi/2)$ though the quasiparticle energy at $(\pi, \pi)$ is only slightly larger. This implies that the magnetic properties of $LaSrCuO$ and $YBaCuO$ are identical right near half-filling. At the first glance, this result seems strange as the hole pockets at $(\pi/2, \pi/2)$ apparently lead to incommensurability which has been observed in neutron scattering experiments only in $LaSrCuO$ [6,10]. However, these experiments were made only deep in the metallic phase when the Fermi surface is large and, in $YBaCuO$, is centered around $(\pi, \pi)$. Recently, we considered [18] the situation when spin stiffness becomes negative while holes still occupy pockets at $(\pi/2, \pi/2)$. We found that the equilibrium static spin configuration is not the planar spiral Shraiman-Siggia phase in which susceptibility is peaked at incommensurate momentum, but rather a noncoplanar configuration which very much resembles the $(\pi, \pi)$ state and differs from it only in the existence of small transverse spiral component of the order parameter, $S_{\perp} \sim O(\sqrt{x})$. For this configuration, the susceptibility still has a dominant peak at $(\pi, \pi)$. In other words, the spin structure adjusts to the negative stiffness of the $(\pi, \pi)$ state in such a way that the peak position of the susceptibility does not change as long as hole occupy pockets at $(\pi/2, \pi/2)$. Notice that this is consistent with the RPA-like analysis by Si et al in the metallic phase as very close to the magnetic transition they found the maximum in the susceptibility at $(\pi, \pi)$ for both types of hole-doped materials. The
transformation of the hole Fermi surface with increasing doping content from small to large one, and the related change in magnetic susceptibility still need to be studied.

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FIGURES

FIG. 1. The RPA series for the total static transverse susceptibility. The first term represents the simple bubble, which is the building block of the ladder. Solid and dashed lines denote valence and conduction fermions, respectively. At half filling, only bubbles which contain one valence and one conduction fermion contribute to transverse susceptibility.