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1995 J. Phys.: Condens. Matter 7 133

(http://iopscience.iop.org/0953-8984/7/1/012)

J. Phys.: Condens. Matter 7 (1995) 133–142. Printed in the UK

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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Received 13 July 1994

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 even 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 favour hole pockets at $(\pi/2, \pi/2)$. We also briefly discuss the tendency towards phase separation.

1. Introduction

The intense interest in understanding the properties of high-temperature superconductors initiated theoretical research on the behaviour 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 behaviour of the antiferromagnetic insulators upon doping has 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 [1]. 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 [2] that if the dispersion of vacancies has a minimum at $(\pm\pi/2, \pm\pi/2)$, then the dopants introduced into a commensurate nearest-neighbour 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 [3, 4, 5] that the values of hopping integrals in electron and hole-doped 214 materials are nearly the same: $t \sim 0.4$ eV, $t' \sim -0.2t$, where t' is the nearest-neighbour hopping. Despite this, the incommensurability upon doping has been found only in LaSrCuO compounds [6] while the dynamical structure factor in the doped NdCeCuO remains peaked at (π, π) [5, 7]. Moreover, experimentally, long-range magnetic

0953-8984/95/010133+10$19.50

order in LaSrCuO disappears even 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 centred 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 (π, π) 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 neighbour 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 (π, π). However, self-energy corrections still favour 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 (π, π). 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 the case of YBaCuO, is centred at (π, π). Notice, however, that cluster calculations for the t–t'–J model reported hole pockets at (π, π) for the same ratios of parameters [5, 11]. If it is actually the case for YBaCuO, the spin dynamics very 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 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 gives rise to a contrasting magnetic behaviour near half filling. Finally, we discuss the tendency towards domain-wall formation upon doping. Our conclusions are presented in section 3.

2. Hubbard model with next-nearest-neighbour hopping

We consider the one-band Hubbard model given by

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} a^\dagger_{i,\sigma} a_{j\sigma} - t' \sum_{\langle i,j' \rangle} a^\dagger_{i,\sigma} a_{j'\sigma} + U \sum_i n_\uparrow n_\downarrow. \tag{1}$$

Here j and j' label the nearest and the next-nearest neighbours, 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, 13, 14, 15, 16, 17, 18], is a good starting point for the calculations close to half filling. Below we mostly restrict ourselves to 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 it to the leading term in the $1/S$ expansion. This mean-field theory is meaningless for the nearest-neighbour 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 non-zero t' eliminates the accidental degeneracy even 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.

2.1. 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., the z component of the spin-density operator

$$S(q) = \tfrac{1}{2}\sum_k a^\dagger_{k+q,\alpha}\sigma_{\alpha,\beta}a_{k,\beta}$$

has a non-zero expectation value at $q = Q_0$. We then use the relation

$$\langle \sum_k a^\dagger_{k+Q,\uparrow}a_{k,\uparrow}\rangle = -\langle \sum_k a'_{k+Q,\downarrow}a_{k,\downarrow}\rangle = \langle S_z\rangle$$

to decouple the quartic term in (1). After decoupling, the quadratic Hamiltonian takes the following form:

$$\mathcal{H}_{\mathrm{MF}} = \sum_k{}' \epsilon^+_k (a^\dagger_{k\sigma}a_{k\sigma} + a^\dagger_{k+Q_0\sigma}a_{k+Q_0\sigma}) + \sum_k{}' \epsilon^-_k (a^\dagger_{k\sigma}a_{k\sigma} - a^\dagger_{k+Q_0\sigma}a_{k+Q_0\sigma})$$
$$-\sum_k{}' \Delta\,\mathrm{sgn}(\sigma)(a^\dagger_{k\sigma}a_{k+Q_0\sigma} + a^\dagger_{k+Q_0\sigma}a_{k\sigma}). \tag{2}$$

Primes to the summation signs indicate that the summation is over the reduced Brillouin zone. We have introduced $\Delta = U\langle S_z\rangle$, $\epsilon_k = -2t(\cos k_x + \cos k_y) - 4t'\cos k_x \cos k_y$, $\epsilon^+_k = (\epsilon_k + \epsilon_{k+Q_0})/2 = -4t'\cos k_x \cos k_y$, $\epsilon^-_k = (\epsilon_k - \epsilon_{k+Q_0})/2 = -2t(\cos k_x + \cos k_y)$. The next step is the diagonalization of the quadratic form by a Bogolyubov transformation

$$a_{k,\sigma} = u_k c_{k\sigma} + v_k d_{k\sigma}\, a_{k+Q_0,\sigma} = \mathrm{sgn}(\sigma)(u_k d_{k\sigma} - v_k c_{k\sigma}). \tag{3}$$

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]:

$$u_k = \left[\frac{1}{2}\left(1 + \frac{\epsilon^-_k}{E^-_k}\right)\right]^{1/2} \qquad v_k = \left[\frac{1}{2}\left(1 - \frac{\epsilon^-_k}{E^-_k}\right)\right]^{1/2} \tag{4}$$

where $E^-_k = \sqrt{\Delta^2 + (\epsilon^-_k)^2}$.

After the diagonalization, equation (2) takes the form

$$\mathcal{H}_{\mathrm{MF}} = \sum_k{}' E^c_k c^\dagger_{k\sigma}c_{k\sigma} - E^d_k d^\dagger_{k\sigma}d_{k\sigma} \tag{5}$$

where

$$E^c = E^-_k + \epsilon^+_k \qquad E^d = E^-_k - \epsilon^+_k. \tag{6}$$

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

$$\frac{1}{U} = \sum_k{}' \frac{1}{E^-_k}. \tag{7}$$

At large U, we obtain, as usual, $\Delta = U/2$, or $\langle S_z\rangle \approx \frac{1}{2}$.

2.2. 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, equation (6), 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-neighbour 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 the t–t'–U model is that at finite t', the degeneracy is removed at the mean-field level. Indeed, a simple inspection of equation (6) 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 [20]. Now, for both 214 compounds, t' is negative and relatively small: $|t'| \sim 0.07$ eV, which is smaller than the exchange integral $J \sim 0.13$ eV [21, 22, 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_k^d and obtain

$$E_k^d = \Delta + \frac{k_\perp^2}{2m_\perp} + \frac{k_\parallel^2}{2m_\parallel} \tag{8}$$

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 the nearest-neighbour 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 $0.25t$ due to quantum fluctuations as was obtained in the $1/S$ expansion for the Hubbard model [17] and in numerical [25] and variational [26] 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 that 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 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. 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 Levin, Si and co-authors [9]. They found that to fit the photoemission data for $YBa_2Cu_3O_7$ [8], one needs $t \sim 0.25$–0.3 eV and a relatively large next-nearest-neighbour hopping term $t' \sim -0.5t$ [9]. The values of the hopping integrals very 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 (6) is nearly degenerate along $k_x = k_y$: the band minima at $t = 0.3$ eV is at (π, π), but the quasiparticle energy at

$(\pi/2, \pi/2)$ is only 0.08 eV 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 $t = 0.3$ eV, we have $\Delta = 4t^2\langle S_z\rangle/J \sim 0.9$ eV [28] and hence $\Delta E \sim 0.8$ eV. This implies that the actual critical value of $|t'|$ above which pockets are located at (π, π), is about 0.32 eV, which is substantially larger than $|t'| \sim 0.13$–0.15 eV 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 the 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 the actual value in in YBaCuO, but, as we already mentioned in section 1, small-cluster calculations for the t–t'–J model found the minimum of hole dispersion at (π, π) 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 behaviour near half filling.

2.3. *Magnetic susceptibility*

In the SDW theory, the spin susceptibility is given by a ladder series of bubble diagrams (figure 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 from the 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

$$\chi^{+-}(q) = \frac{\chi_0(q)}{1 - U\chi_0(q)} \tag{9}$$

where

$$\chi_0^{+-}(q) = \frac{1}{2N}\sum_{E^d > |\mu|}{}' \left[1 - \frac{\epsilon_k^- \epsilon_{k+q}^- - \Delta^2}{E_k^- E_{k+q}^-}\right]\left(\frac{1}{E_k^c + E_{k+q}^d} + \frac{1}{E_k^d + E_{k+q}^c}\right)$$
$$+\frac{1}{N}\sum_{\substack{E_{k+q}^d > |\mu| \\ E_k^d < |\mu|}}{}' \left[1 + \frac{\epsilon_k^- \epsilon_{k+q}^- - \Delta^2}{E_k^- E_{k+q}^-}\right]\frac{1}{E_{k+q}^d - E_k^d}. \tag{10}$$

Above we have 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 (π, π) in accordance with the Goldstone theorem. Near this point, the static susceptibility has the form [30]

$$\chi^{+-}(q) = \frac{2N_0^2}{\rho_s(q - Q_0)^2} \tag{11}$$

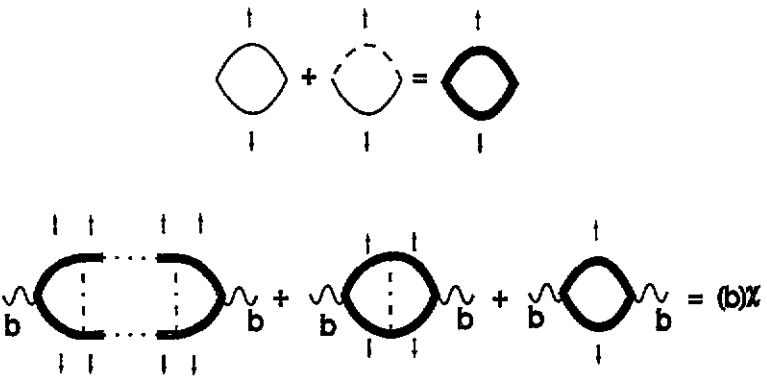

Figure 1. The RPA series for the total static transverse susceptibility. The first term represents the simple bubble, which is the building block of the ladder. Solid and dashed lines denote valence and conduction fermions, respectively. At half filling, only bubbles which contain one valence and one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

where N_0 is the sublattice magnetization ($= \frac{1}{2}$ in our mean-field approach), and ρ_s is the spin stiffness which should be positive.

Let us first consider half filling. Here only the first term contributes to χ_0. Performing an expansion in (10) and substituting the result into (9), we obtain the 'classical' spin wave result

$$\rho_s = \frac{1}{4} J \left(1 - \frac{2(t')^2}{t^2}\right). \tag{12}$$

Clearly then, the commensurate (π, π) 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 (π, π) and combining the result with (12), we obtain

$$\rho_s(\delta) = \rho_s(0)(1 - z) \tag{13}$$

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

$$z = 4U \frac{1}{N} \lim_{q \to 0} \sum_{\substack{E^d_{k+q} > |\mu| \\ E^d_k < |\mu|}}{}' \frac{\sin^2 k_x}{E^d_{k+q} - E^d_k}. \tag{14}$$

At small concentration of holes, the condition $E^d_k < |\mu|$ 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

$$z = 2U_{\text{eff}} \frac{\sqrt{m_\perp m_\parallel}}{\pi}. \tag{15}$$

For the case of $(\pi/2, \pi/2)$ pockets, $|t'| \leqslant J$, 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 (π, π) antiferromagnetic state becomes unstable. In more sophisticated calculations however, U_{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_{eff} yields $U_{\text{eff}} \sim J$ at $U \gg t$, and therefore $z \sim \text{O}(1)$ [2, 31, 16]. In any event, however, it is likely that z can be 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 $(0, \pi)$. Equations (13) and (14) are still valid, but the numerator in (14) now vanishes right at the centre 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, ρ_s acquires only a small correction $\text{O}(\delta)$. Clearly then, antiferromagnetism at (π, π) 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 a 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 disordering transition at least in LaSrCuO is in the universality class of the non-linear sigma model, and has the dynamical exponent $\bar{z} = 1$ [32] (the most direct evidence is the observed linear behaviour of the uniform susceptibility). This implies that in a more adequate model, the decrease in ρ_s must eventually lead to a 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 one range of the coupling-constant values. In another range, he found an incommensurate transition within the ordered phase as in our approach. It is essential, however, that the two scenarios differ primarily in the behaviour 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 the large-S expansion, as in our approach) the smaller is the actual region of the magnetically ordered phase. If these arguments are accepted, then the width of 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 that 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 short-ranged local distortions in NdCeCuO and long-ranged distortions in LaSrCuO, was presented in [5].

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

2.4. Phase separation

In the SDW approach, we can also consider the stability of the (π, π) phase at small doping against the formation of domain walls [34, 35]. This stability requires the longitudinal spin susceptibility to be positive. For 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 χ^{zz} can be obtained by straightforward manipulations starting from equations (52)–(54) in [16]:

$$\chi^{zz} \approx \frac{2\chi^{\text{Pauli}}}{1 - 8J\chi^{\text{Pauli}}} \tag{16}$$

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), but is much weaker in YBaCuO where the Pauli susceptibility is about two times smaller. At the same time, we found that the denominator in χ^{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 [5]. This paper also pointed to the possibility of two-dimensional phase separation in the electron-doped materials which we have not studied.

3. Conclusions

To summarize, in this paper we presented simple calculations which show that the stability of the commensurate antiferromagnetic state in 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, even 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 behaviour 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 [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 (π, π) is only slightly larger. This implies that the magnetic properties of LaSrCuO and YBaCuO are identical very near half filling. On 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 performed only deep in the metallic phase when the Fermi surface is large and, in the case of YBaCuO, crosses the Brillouin zone boundary thus giving rise to damping of spin waves into a particle–hole continuum. As regards incommensurability in the ordered state, we recently considered [18] the equilibrium

static spin configuration for $z > 1$ and found that it is not the planar spiral Shraiman–Siggia phase in which susceptibility is peaked at incommensurate momentum, but rather a non-coplanar configuration which very much resembles the (π, π) state and differs from it only in the existence of a *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 (π, π). In other words, the spin structure adjusts itself to a negative stiffness of the (π, π) state in such a way that the peak position of the susceptibility does not change as long as holes occupy pockets at $(\pi/2, \pi/2)$. Notice that this result is consistent with the RPA-like analysis by Si *et al* [9] in the metallic phase, as very close to the magnetic transition they found the maximum in the susceptibility at (π, π) for both types of hole-doped material. The transformation of the hole Fermi surface with increasing doping content from small to large, and the related change in magnetic susceptibility, still has to be studied in detail.

Acknowledgments

It is our pleasure to thank E Dagotto, D Frenkel, R J Gooding, R Joynt, and Q Si for useful conversations. We are also grateful to R J Gooding and E Dagotto for sending us copis of [5] and [25] prior to publication. The research was supported in part by the Graduate School at the University of Wisconsin—Madison and the Electric Power Research Institute.

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