

Theory of electron-hole asymmetry in doped CuO_2 planes

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The magnetic phase diagrams, and other physical characteristics, of the hole-doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and electron-doped $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ high-temperature superconductors are profoundly different. Given that it is envisaged that the simplest Hamiltonians describing these systems are the same, viz., the t - t' - J model, this is surprising. Here we relate these physical differences to their ground states' single-hole quasiparticles, the spin distortions they produce, and the spatial distribution of carriers for the multiply doped systems. As is well known, the low doping limit of the hole-doped material corresponds to $\mathbf{k} = (\frac{\pi}{2}, \frac{\pi}{2})$ quasiparticles, states that generate so-called Shraiman-Siggia long-ranged dipolar spin distortions via backflow. These quasiparticles have been proposed to lead to an incommensurate spiral phase, an unusual scaling of the magnetic susceptibility, as well as the scaling of the correlation length defined by $\xi^{-1}(x, T) = \xi^{-1}(x, 0) + \xi^{-1}(0, T)$, all consistent with experiment. We suggest that for the electron-doped materials the single-hole ground state corresponds to $\mathbf{k} = (\pi, 0)$ quasiparticles; we show that the spin distortions generated by such carriers are shortranged. Then, we demonstrate the effect of this single-carrier difference in many-carrier ground states via exact diagonalization results by evaluating $S(\mathbf{q})$ for up to four carriers in small clusters. Consistent with experiment, for the hole-doped materials short-ranged incommensurate spin orderings are induced, whereas for the electron-doped system only commensurate spin correlations are found. Further, we propose that there is an important difference between the spatial distributions of mobile carriers for these two systems: for the hole-doped material the quasiparticles tend to stay far apart from one another, whereas for the electron-doped material we find tendencies consistent with the clustering of carriers, and possibly of low-energy fluctuations into an electronic phase-separated state. Phase separation in this material is consistent with the midgap states found by recent angle-resolved photoemission spectroscopy studies. Last, we propose the extrapolation of an approach based on the t - t' - J model to the hole-doped 123 system.

I. INTRODUCTION

The CuO_2 plane-based high-temperature superconductors have anomalous normal state properties. One part of the normal state puzzle involves the spin orderings, and for the majority of this paper we focus on the differing magnetic phase diagrams for the hole-doped Bednorz-Müller $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ compounds¹ in comparison to the electron-doped $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ materials.² In particular, for both of these systems the $x = 0$ phase possesses three-dimensional antiferromagnetic long-ranged order.^{3,4} However, one must heavily dope the Nd compound to destroy this order, say, $\sim 12\%$, while only a small doping of $\sim 2\%$ is required to eliminate long-ranged antiferromagnetic order in the La cuprate material. A schematic of the contrasting phase diagrams is given in Fig. 1.

One important aspect of the magnetic orderings found in these systems involves the kinds of spin correlations that these systems exhibit when doped to levels greater than 2%. As mentioned above, for the electron-doped material antiferromagnetic order persists until $\sim 12\%$ doping levels are reached. However, when the hole-doped

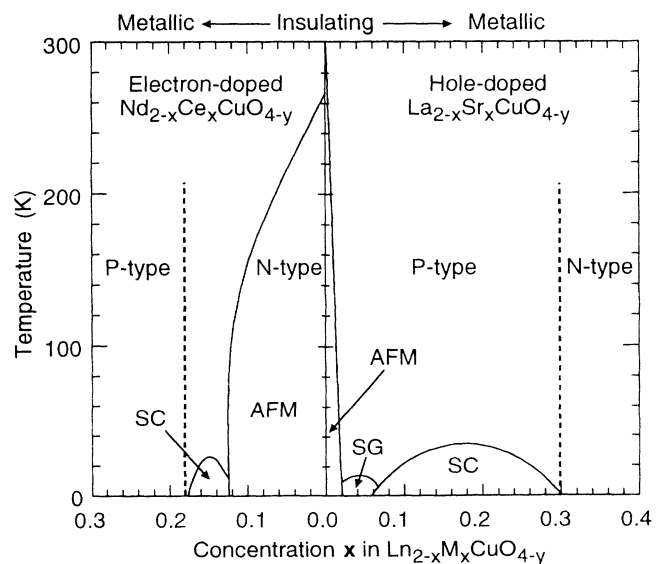


FIG. 1. A schematic of the phase diagrams, as a function of temperature and doping concentrations away from half filling, for both the hole- and electron-doped materials (after Ref. 36, from Ref. 4).

system has say 7% holes in a CuO_2 plane, short-ranged incommensurate magnetic ordering is found. This appears experimentally in the dynamic magnetic response, and has been found via inelastic neutron scattering for a number of intermediate doping levels.⁵⁻⁷ Consequently, an alternate way in which one can phrase the question concerning the differing magnetic phase diagrams is, why does the electron-doped system maintain commensurate antiferromagnetic order at doping levels that induce incommensurate correlations in the hole-doped system?

Several theories have addressed the phase diagrams of these doped antiferromagnetic insulators. When the La-based system is doped, the carriers predominantly occupy O sites, in particular as O^- states, whereas for the Nd-based material the carriers are believed to be associated with the addition of an electron to a Cu $3d^9$ ion, thus forming Cu^+ . Then, a common explanation of these differing magnetic phase diagrams follows from the assumption of the complete localization of the carriers, and the ensuing spin distortions generated by such static defects. Namely, (i) the dramatic reduction of the Néel temperature $T_N(x)$ in the hole-doped system results from frustrating ferromagnetic bonds being embedded in an antiferromagnetic background, the so-called Aharony model.⁸ Such frustrated bonds generate a long-ranged spin distortion with dipolar symmetry, and numerical studies⁹ have shown that a version of this perturbation renormalized by quantum fluctuations^{9,10} indeed alters the spin-spin correlation length in a fashion consistent with experiment.¹¹ (ii) Fixed Cu^+ sites in a background antiferromagnetic lattice act like static vacancies, and subsequently diminish the spin-wave stiffness¹² in a manner consistent with experiment.¹³ Monte Carlo studies of this quantum dilution problem^{12,14} do not suffer from the minus sign problem, and thus are capable of accurately characterizing the spin correlation length.

Unfortunately, these cannot be complete explanations of the differing magnetic phase diagrams. Near the antiferromagnetic phase boundary (temperature vs doping) the carriers are mobile in both of these systems,^{15,16} and thus one must come to an understanding of the differing reductions of the spin orderings for mobile, not just localized, carriers. This is one of the focuses of this paper.¹⁷

Here we put forward a proposal explaining the electron-hole asymmetry of the magnetic phase diagrams shown in Fig. 1 for mobile carriers. Our work builds on our earlier study¹⁸ that showed that for the t - J model and the hole-doped system, a tendency towards short-ranged incommensurate order vs hole doping arises. The results of Ref. 18 are consistent with experiment,⁵⁻⁷ and in part is further verification of earlier exact diagonalization work of Moreo *et al.*,¹⁹ as well as Monte Carlo work.^{20,21} However, the important point of Ref. 18 was that this incommensurability only occurred for the single-hole system having a ground state momentum of $\mathbf{k} = \pm(\frac{\pi}{2}, \pm\frac{\pi}{2})$ [since $\mathbf{k} = (\frac{\pi}{2}, \frac{\pi}{2})$ quasiparticles generate long-ranged spin distortions similar to those produced by a ferromagnetic bond, the success of the above-mentioned Aharony model bodes well for any theory predicting that these carriers exist in the hole-doped 214 systems]. If the momentum of the single-hole ground state is $\mathbf{k} = (\pi, 0)$,

something that may be accomplished through the use of the t - t' - J model (see below) with $t'/t > 0$, then the tendency towards incommensurability is eliminated and only commensurate ordering remains. Clearly, this is similar to the above-mentioned behavior of the hole- and electron-doped materials, and in this paper we will make this comparison complete.

Very shortly after Ref. 18, Tohyama and Maekawa²² also studied the t - t' - J model, now for the electron- and hole-doped systems. They suggested, consistent with a considerable amount of electronic structure work,²³⁻²⁵ as well as angle-resolved photoemission spectroscopy (ARPES) results for the electron-doped system,²⁶ that the Nd system corresponded to hopping integrals t and t' with (approximately) just-flipped signs in comparison to the same hopping integrals believed to be appropriate for the hole-doped materials (we elaborate on this relation in the next section). Then, by examining the energy to the first excited states, they demonstrated that the commensurate antiferromagnetic order was much more stable for the electron-doped system than for the hole-doped systems. As we show below, this is complementary to our work in Ref. 18, since the single-hole ground state momentum for their electron-doped t - t' - J Hamiltonian is actually $\mathbf{k} = (\pi, 0)$. We then strengthen the arguments of Tohyama and Maekawa by evaluating the magnetic structure factor $S(\mathbf{q})$ for the many-carrier ground states for these two systems. Indeed, using the relevant material parameters, we find incommensurate ordering tendencies for the hole-doped material, while for the electron-doped material the magnetic ordering is always commensurate, in complete agreement with experiment.

We shall also be concerned with other physical properties of the hole- and electron-doped materials. For the La cuprates, some experiments can be explained beginning with the assumption that at low doping level Shraiman-Siggia²⁷ dipolar quasiparticles are present (implicit in these theories is the existence of hole pockets, or a "small" Fermi surface, something that so far has not been observed). One such magnetic problem involves the scaling of the correlation length with doping and temperature, viz., $\xi^{-1}(x, T) = \xi^{-1}(x, 0) + \xi^{-1}(0, T)$, and this has been found to be reproduced by a model (based on the existence of these dipolar quasiparticles) proposed by one of us²⁸ for both mobile and localized carriers, and is in close agreement with experiment.¹¹ Further, a theory²⁹ of the temperature- and doping-dependent magnetic susceptibility $\chi(x, T)$ has been found to be consistent with experiment.³⁰ Last, the same theory³¹ also predicts the existence of a pseudogap, something that may be consistent with experiment.³²

We are proposing that these dipolar quasiparticles do not exist in the weakly doped Nd cuprates, and thus, e.g., $\xi(x, T)$, $\chi(x, T)$, and the optical properties of this system may be quite different from those of the La cuprates. Unfortunately, the collection of experiments performed on the electron-doped materials is not as complete as the set performed for the hole-doped system, and so a full comparison is not possible. However, there is one striking difference between the normal state properties of these systems, and that is the resistivities at optimal

doping. The La system shows a linear- T resistivity,¹⁵ whereas the Nd system shows a clear Fermi-liquid-like T^2 dependence.³³ Another intriguing experimental result for the electron-doped material corresponds to the midgap states seen in the angle-integrated photoemission work of Anderson *et al.*²⁶ It has been proposed³⁴ that this is a signal of phase separation, and to this end we have examined the spatial distributions of many carriers, as well as measured the interaction energies between carriers. Our results tend to support a phase separation hypothesis, but *only* for the electron-doped system.

Our paper is organized as follows. In Sec. II we discuss the formal aspects of the t - t' - J model and display the electron-hole symmetries and asymmetries that can be identified when these materials are doped away from half filling. In Sec. III we summarize previously published and our recent exact diagonalization results for the one-carrier ground states for these two systems, and show that these two systems have different one-carrier ground states. Then, the spin correlations found in $S(\mathbf{q})$ as a function of doping are shown to be in agreement with the phase diagram of Fig. 1. In Sec. IV we examine the spin distortions produced by each of these quasiparticles via our semiclassical analysis of this Hamiltonian for a single carrier; this will be shown to agree with the exact diagonalization results. Quantum fluctuations are shown to not affect these conclusions. Then we examine the spatial distribution of carriers pointing out the acute difference between the hole- and electron-doped systems — from this we relate the tendency towards clustering of carriers of the electron-doped system to the midgap states seen in photoemission. Finally, in Sec. V we discuss the relevance of our results to the transport properties of both kinds of systems, and as a prelude to possible future work we consider the extrapolation of this approach to other systems, and in particular consider the commensurability that persists in the hole-doped Y-Ba-Cu-O system.

II. t - t' - J MODEL

A. Electron-hole asymmetry induced by t'

We begin our discussion of the t - t' - J model by first considering a simpler model involving only hopping terms to the nearest- and next-nearest-neighbor sites along a one-dimensional chain — this model provides the most direct demonstration of the electron-hole asymmetry about half filling that t' introduces into the problem.

Consider a linear chain with a single orbital per site, and define the vacuum to be the state with all orbitals devoid of electrons. Introduce

$$H_{\text{hop}} = -t \sum_{\langle i,j \rangle_{\text{NN}} \sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.} \right) - t' \sum_{\langle i,k \rangle_{\text{NNN}} \sigma} \left(c_{i\sigma}^\dagger c_{k\sigma} + \text{H.c.} \right), \quad (2.1)$$

where $\langle \rangle_{\text{NN}}$ denotes nearest neighbors, $\langle \rangle_{\text{NNN}}$ next-nearest neighbors, and $c_{i\sigma}$ is the electron annihilation

operator for site i and spin σ (note that these operators are *not* constrained to prohibit double occupancy — see Sec. II B). Then imagine that the system has an up spin at every site except one, at which no electron is present. The energy eigenvalues for this hole plus spin-polarized background are given by

$$E(k) = -2t \cos(k) + 2t' \cos(2k) \quad (\text{hole}). \quad (2.2)$$

Now consider a system with up spins at every site, and that in addition to these electrons one down-spin electron is placed in some orbital. Then the energy eigenvalues of this composite spin-polarized plus mobile electron system are

$$E(k) = -2t \cos(k) - 2t' \cos(2k) \quad (\text{electron}). \quad (2.3)$$

From these results it is to be noted that while the near-neighbor hopping leads to identical energies for both the hole- and electron-doped systems, the next-nearest-neighbor hopping has different signs. This reflects the breaking of electron-hole symmetry that t' induces, and thus its inclusion in our starting Hamiltonian is crucial. It is to be stressed that this asymmetry is found in any dimension, for any spin background, but only for doping levels close to half filling.

B. Strong-coupling Hamiltonian

Equation (2.1) is not a good starting point for describing the physics of the CuO₂ planes in either La-Sr-Cu-O or Nd-Ce-Cu-O, since it only describes free carriers. If instead one begins with an extended Hubbard model description³⁵ of the strong correlation effects known to be present in these systems, and then examines the systems at close to half filling, one can obtain the so-called t - t' - J model.³⁶ To be specific, one considers

$$H = -t \sum_{\langle i,j \rangle_{\text{NN}} \sigma} \left(\tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + \text{H.c.} \right) - t' \sum_{\langle i,k \rangle_{\text{NNN}} \sigma} \left(\tilde{c}_{i\sigma}^\dagger \tilde{c}_{k\sigma} + \text{H.c.} \right) + J \sum_{\langle i,j \rangle_{\text{NN}}} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j), \quad (2.4)$$

where J is the Heisenberg superexchange constant coupling spins \mathbf{S}_i between nearest-neighbor sites. Also, in Eq. (2.4) constrained electron operators are used (constrained to disallow double occupancy at any site), viz.,

$$\tilde{c}_{i\sigma} = c_{i\sigma} (1 - c_{i-\sigma}^\dagger c_{i-\sigma}) . \quad (2.5)$$

We wish to stress that our use of the t - t' - J model is based on beginning with a three-band extended Hubbard model description³⁵ for *both* the La-Sr-Cu-O and Nd-Ce-CuO systems. While it is well known³⁷⁻³⁹ that for the hole-doped systems one may approximately map the three-band Hubbard model onto the one-band t - t' - J model (N.B. not necessarily the one-band Hubbard model), it may be argued that this is also the correct starting point for the electron-doped systems. For example, the dominant contribution to the t' hopping integral for the electron-doped system is *not* due to a di-

rect Cu-Cu overlap, but rather follows from a third-order $\text{Cu} \rightarrow \text{O} \rightarrow \text{O} \rightarrow \text{Cu}$ hopping.⁴⁰ Thus, in what follows we consider (i) the t and t' parameters that are to be *fitted* via quantum cluster studies (see below), and not due to a strong-coupling mapping of the one-band Hubbard model onto a Hilbert space prohibiting double occupancy,⁴¹ and (ii) the superexchange constant J to be found from either quantum cluster studies, or from comparison to experiments probing the magnetic structure and/or excitations.

In the previous subsection we were able to treat hole- and electron-doped systems with the same starting Hamiltonian. However, now it is clear that the above Hamiltonian, for a vacuum corresponding to no electrons at any site, cannot be used to describe both hole and electron doping of the half-filled state. For example, a vacancy can easily be added to a spin-polarized ferromagnetic state, and is completely mobile, while a down-spin electron added to such a spin background is completely localized. Consequently, with this Hamiltonian and this vacuum, only hole-doped CuO_2 planes may be investigated.

To investigate the electron-doped system it is usual to introduce an electron-hole transformation, viz.,

$$c_{i\sigma} \rightarrow a_{i\sigma}^\dagger, \quad (2.6)$$

where $a_{i\sigma}$ is the annihilation operator of a hole at site i of spin σ . (With this transformation it follows that one now considers a vacuum with no holes at any site.) However, this does not lead to the desired Hamiltonian as one finds that the new hopping term does not describe constrained (viz., two holes are never allowed on the same site) hopping. Instead, one must utilize a more general model than Eq. (2.4), one that includes so-called doublon hopping processes,⁴² and from this starting Hamiltonian it is straightforward to derive the required transformation. The result of this transformation can then be shown to be equivalent to

$$\tilde{c}_{i\sigma} \rightarrow \tilde{a}_{i\sigma}^\dagger, \quad (2.7)$$

where the $\tilde{a}_{i\sigma}$ also satisfy fermionic anticommutation relations. Thus, one eventually finds that the appropriate t - t' - J model for the electron-doped system is the same as Eq. (2.4) but with the $\tilde{a}_{i\sigma}$ replacing the $\tilde{c}_{i\sigma}$ and with the minus signs in front of t and t' changed to be plus signs.

Summarizing the above discussion, the t - t' - J Hamiltonian will be used to model the physical systems that we are interested in. We consider this model to possess the bare minimum number of processes through which both the hole- and electron-doped CuO_2 planes can be represented. To be specific, (i) Eq. (2.4) with a vacuum of zero electrons at every site of a square lattice will describe the hole-doped system, and (ii) for the electron-doped systems we use

$$\begin{aligned} H = & t \sum_{\langle i,j \rangle_{\text{NN}\sigma}} \left(\tilde{a}_{i\sigma}^\dagger \tilde{a}_{j\sigma} + \text{H.c.} \right) \\ & + t' \sum_{\langle i,k \rangle_{\text{NNN}\sigma}} \left(\tilde{a}_{i\sigma}^\dagger \tilde{a}_{k\sigma} + \text{H.c.} \right) \\ & + J \sum_{\langle i,j \rangle_{\text{NN}}} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j). \end{aligned} \quad (2.8)$$

For this latter Hamiltonian we use a vacuum of zero holes at every site of a square lattice. Thus, note that, quite simply, in comparison to the hole-doped Hamiltonian the signs of the t and t' hopping terms are flipped and the \tilde{a} operators replace the \tilde{c} operators. Thus, from now on we simply use Eq. (2.4) for both systems, specifying $t = 1$ for hole doping, and $t = -1$ for electron doping.²²

We now consider the numerical values of the hopping and superexchange parameters. A consequence of the holes residing on the O sites in the La material is that for a quantitative determination of the hopping parameters t and t' , something very different from overlap integrals must be evaluated. We refer the interested reader to the summary of this problem given by Tohyama and Maekawa,²² and simply state the range of accepted values.²²⁻²⁴ For the hole-doped La-Sr-Cu-O system, using Eq. (2.4), one may scale all energies such that $t = 1$. Then one has $J \approx 0.3 \rightarrow 0.4$ and $t' \approx -0.2 \rightarrow -0.4$. For the electron-doped Nd-Ce-Cu-O system we again use Eq. (2.4) but now with $t = -1$, and $J \approx 0.3 \rightarrow 0.4$ and $t' \approx +0.2 \rightarrow +0.4$. Thus, it is interesting to note that even though a Zhang-Rice singlet is not exactly equivalent to a Cu $3d^8$ ion, the material parameters for these two systems are such that the electron-hole mapping given in Eq. (2.7) predicts reasonably well the numerical values that one must employ for one system given the parameters of the other.

III. NUMERICAL RESULTS

Stephan and Horsch⁴³ have proposed that knowledge of the single-hole system does not lead to valuable information on the multiply doped state. In Ref. 18 we showed that this is not always the case, and that, in particular, knowledge of the one-hole ground state can aid in predicting the presence or absence of incommensurate correlations. Thus, we begin a discussion of our numerical work with a summary of the single-hole ground state.

There has already been a comprehensive exact diagonalization study of the ground state of one hole in the t - t' - J model for a 4×4 square cluster in Ref. 44 (since they use a bosonic representation, their sign of t' is flipped in comparison to ours). For the physically relevant ratio of J/t they find a $\mathbf{k} = \pm(\frac{\pi}{2}, \pm\frac{\pi}{2})$ ground state when the t' corresponding to hole-doped materials is used (unless $|t'|$ becomes too large), and a $\mathbf{k} = \pm(\pi, 0), \pm(0, \pi)$ ground state for the t' associated with the electron-doped materials.

We have used a Lanczos routine and have also performed exact diagonalization evaluations⁴⁵ of the ground states of the t - t' - J model for $J = 0.4$, with $t = \pm 1$ for $t' = \pm 0.1, \pm 0.2$, and ± 0.3 . For the conventional 4×4 16-site square cluster our work agrees with that of Ref. 44. We have also studied the $\sqrt{8} \times \sqrt{32}$ 16-site cluster introduced in Ref. 18, as well as some results generated using a $\sqrt{18} \times \sqrt{32}$ 24-site cluster.⁴⁶ For the hole-doped material, viz., when $t' < 0$, we always find a ground state of $\mathbf{k} = \pm(\frac{\pi}{2}, \pm\frac{\pi}{2})$, while for the electron-doped material, viz., when $t' > 0$, we always⁴⁸ find a ground state of $\mathbf{k} = (\pm\pi, 0), (0, \pm\pi)$. Our results for these two different

clusters are entirely consistent with the phase diagram of Ref. 44 found using the 4×4 cluster.

Our numerical results also lead us to expect that the band structures for the hole- and electron-doped materials will be quite different. We find that the band structure of the hole-doped material is similar to Fig. 4 of Ref. 18 (which is a $t' = 0$ curve), although with the increased ratio of $|t'/t|$ that we are using here the band along $\mathbf{k} = (0, 0) \rightarrow (\pi, 0)$ becomes quite flat. This is similar to recent photoemission work of the valence band of undoped $\text{Sr}_2\text{CuO}_2\text{Cl}_2$,⁴⁹ and provides some experimental support for a value of t' around $-0.3t$. We have listed the single-carrier band structure energies for our $\sqrt{18} \times \sqrt{32}$ 24-site cluster in Table I for both the hole- and electron-doped systems having used $t'/t = -0.3$.

The single-hole ground states of the hole- and electron-doped materials are different — so what? As mentioned above, the important fact contained in Ref. 18 is that a knowledge of the single-hole ground state can aid in understanding whether or not any short-ranged incommensurate correlations are introduced into the ground state of the multiply doped system. This followed from (i) if the single-hole ground state is not a $\mathbf{k} = \pm(\frac{\pi}{2}, \pm\frac{\pi}{2})$ state, no tendencies towards incommensurate correlations occurred, consistent with the spiral phase prediction of Shraiman and Siggia,⁵⁰ and (ii) the electron momentum distribution function for 2, 3, and 4 holes was found to be composed of the half-filled Fermi surface with dimples at those momenta corresponding to the single-hole ground states, thus suggesting that some form of rigid band filling¹⁸ is in effect. Combining this with the differing single-hole ground states mentioned above, it is clear that we can now extrapolate these abstract results to the physical systems under consideration.

Figures 2 and 3 show the magnetic structure factor for 0, 1, 2, 3, and 4 holes (electrons) for $t' = \pm 0.3$ evaluated with the $\sqrt{8} \times \sqrt{32}$ cluster introduced in Ref. 18 — similar results are obtained for other $\pm t'$ pairs. For the hole-doped material, Fig. 2 displays that the peak in the structure factor shifts from (π, π) for 0 and 1 hole, to $(\frac{3\pi}{4}, \frac{3\pi}{4})$ for 2 holes, to $(\frac{\pi}{2}, \frac{\pi}{2})$ for 3 and 4 holes. This

TABLE I. Single-carrier minimum energies for both hole and electron singly doped planes, described by Eq. (2.4), for the allowed wave vectors of our nonsquare 24-site cluster. All energies are in units of t .

\mathbf{k}	Energy	Energy
	(Hole doped: $t = 1, t' = -0.3$)	(Electron doped: $t = -1, t' = +0.3$)
$(0, 0)$	-12.824	-12.153
$(\frac{\pi}{4}, \frac{\pi}{4})$	-12.961	-12.338
$(\frac{\pi}{2}, \frac{\pi}{2})$	-13.207	-12.686
$(\frac{3\pi}{4}, \frac{3\pi}{4})$	-13.063	-12.375
(π, π)	-12.853	-12.177
$(\frac{-\pi}{3}, \frac{\pi}{3})$	-12.997	-12.471
$(\frac{-2\pi}{3}, \frac{2\pi}{3})$	-13.127	-12.363
$(\frac{-\pi}{12}, \frac{7\pi}{12})$	-12.896	-12.746
$(\frac{-5\pi}{12}, \frac{11\pi}{12})$	-12.980	-12.679
$(\frac{\pi}{6}, \frac{5\pi}{6})$	-12.821	-13.037

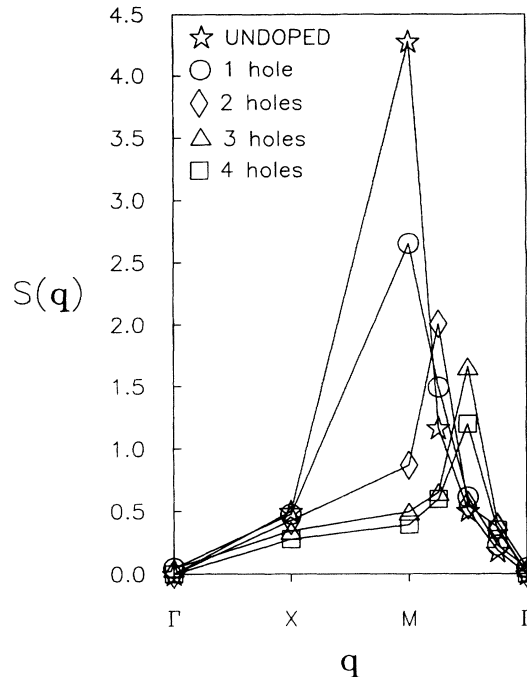


FIG. 2. The magnetic structure factor for the t - t' - J model given in Eq. (2.4) for 0, 1, 2, 3, and 4 carriers; here, the carriers are mobile holes. For this figure, $t = +1$, $t' = -0.3$, and $J = 0.4$, which are appropriate for hole-doped La-Sr-Cu-O. The reciprocal lattice points are as follows: $\Gamma = (0, 0)$, $X = (\pi, 0)$, and $M = (\pi, \pi)$.

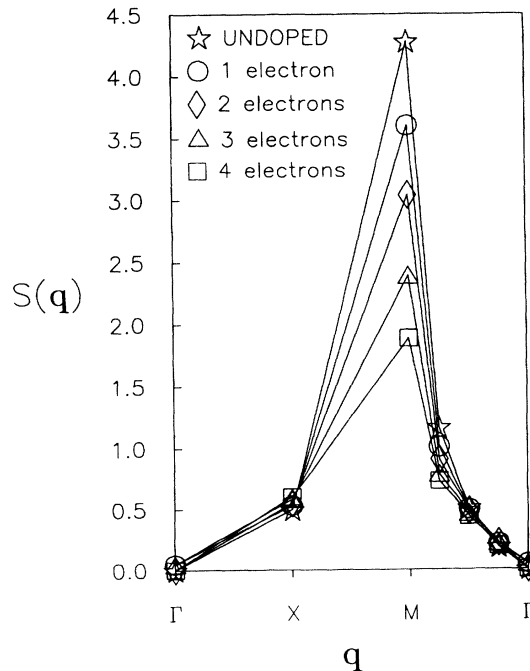


FIG. 3. The magnetic structure factor for the t - t' - J model given in Eq. (2.4) for 0, 1, 2, 3, and 4 carriers; here, the carriers are mobile electrons. For this figure, $t = -1$, $t' = +0.3$, and $J = 0.4$, which are appropriate for electron-doped Nd-Ce-Cu-O.

behavior is similar to the behavior displayed in Fig. 5 of Ref. 18 for $t' = 0$. However, in Fig. 3 it is seen that no shifts of the maximum of $S(\mathbf{q})$ away from (π, π) occurs for any doping concentration away from half filling for the electron-doped system. These results are entirely consistent with Fig. 1, and, in particular, are consistent with the lack of any tendency of the electron-doped materials to display the kind of incommensurate correlations that are present in the hole-doped system.⁵¹ Clearly, these numerical results suggest that we have found a reasonable starting point from which one can hope to be able to describe the hole- and electron-doped 214 systems. We now try to come to an understanding of these numerical results.

IV. ANALYSIS

As mentioned in the Introduction, the existence of Shraiman-Siggia quasiparticles in weakly doped La-Sr-Cu-O is supported by the theories^{9,28,29,31,52} that assume their existence, and are subsequently able to produce results consistent with experiment. To be specific, it seems that a scenario in which these quasiparticles are weakly interacting and tend to stay very far apart from one another (thus making it likely that some form of rigid band filling [e.g., with hole pockets around $\pm(\frac{\pi}{2}, \pm\frac{\pi}{2})$]) is applicable.

Now we study the $(\pi, 0)$ quasiparticles: We are proposing that these are the single-hole ground state constituents that exist in the weakly doped Nd-Ce-Cu-O system. We wish to characterize the spin distortions that each such quasiparticle produces, as well as come to an understanding of the spatial distribution for a state which is multiply doped. This will allow us to (i) understand why the $(\pi, 0)$ and $(\frac{\pi}{2}, \frac{\pi}{2})$ quasiparticles lead to differing magnetic structure factors vs doping, and (ii) examine some of the other physical features that are known to be specific to the electron-doped system.

According to the semiclassical theory of Shraiman and Siggia,²⁷ for ground states with these wave vectors, differing distortions of the spin background occur. For the $\mathbf{k} = (\frac{\pi}{2}, \frac{\pi}{2})$ states, long-ranged spin distortions with dipolar symmetry are produced via backflow. For the $\mathbf{k} = (\pi, 0)$ ground states, the hydrodynamic theory of Shraiman and Siggia²⁷ leads to the prediction that the spin distortion induced by one $(\pi, 0)$ quasiparticle is short ranged. These ideas are verified in our Figs. 4 and 5 where our results from evaluating the energies at this wave vector for the t - t' - J model with the electron-doped material parameters using a semiclassical variational wave function, such as that described in Ref. 27, are displayed. To be specific, we utilize a product state of classical spins in an infinite lattice, and incorporate a broken antiferromagnetic symmetry in calculations of the hopping matrix elements for a single hole (see Ref. 27 for the details of such a variational wave function). Then, to display the range of the spin distortions for this ground state we have calculated the minimum energy as a function of the number of spins away from the hole that are allowed to be distorted from their undoped Néel config-

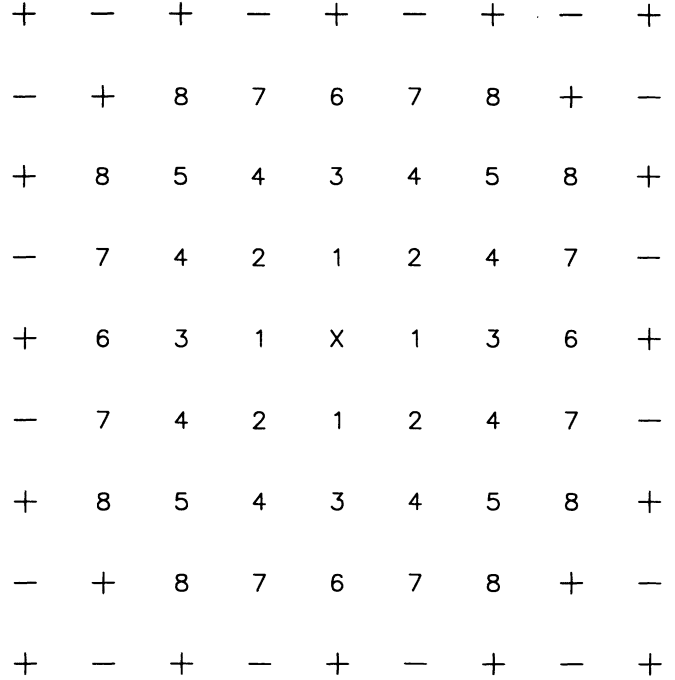


FIG. 4. A picture of the equivalent sites that we allow to be distorted away from their ordered Néel configuration in our calculation of the semiclassical wave function for the t - t' - J model for one carrier. The clusters used in such calculations are infinite in extent.

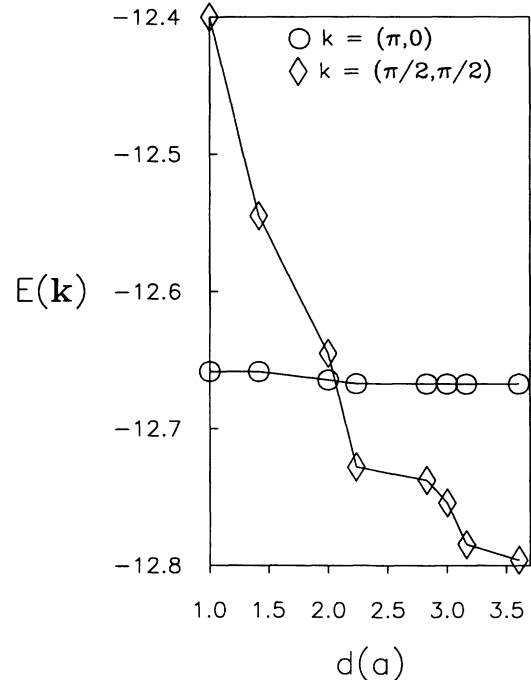


FIG. 5. The energies of the $\mathbf{k} = (\pi, 0)$ ground state for the electron-doped system ($t = -1$, $t' = +0.3$, $J = 0.4$) and the $\mathbf{k} = (\frac{\pi}{2}, \frac{\pi}{2})$ ground state for the hole-doped system ($t = +1$, $t' = -0.3$, $J = 0.4$) obtained via application of the variational principle to a Shraiman-Siggia semiclassical wave function. These energies are found by allowing all spins up to distance d , given in units of the lattice constant a , to be distorted away from their antiferromagnetically aligned state.

uration — these sites are shown in Fig. 4, where they are labeled according to the equivalent sites around a single carrier. In Fig. 5 we show the minimum energies found from the variational principle as a function of these site labels for both the hole-doped $\mathbf{k} = (\frac{\pi}{2}, \frac{\pi}{2})$ one-hole ground state, and the $\mathbf{k} = (\pi, 0)$ electron-doped one-carrier ground state. The long-ranged spin distortion of the hole-doped ground state is clear, whereas the short-ranged distortion of the electron-doped ground state is made manifest by the insensitivity of the minimum energy when one allows more distant neighbors to be distorted from their Néel state.

The above procedure may be repeated for all wave vectors for both hole- and electron-doped Hamiltonians. We find that providing t' satisfies certain inequalities (which necessarily depend on the ratio of J/t) the semiclassical band structure largely reproduces the band structures determined by exact diagonalization. Specifically, the ground states are reproduced when (i) $t' > -0.12$ for the hole-doped material, and (ii) $t' > +0.12$ for the electron-doped materials (these inequalities will be affected by quantum fluctuations — see below). This agreement with the quantum cluster studies provides further evidence that the renormalized classical description of the spin background (*not* including the charge carriers) of the weakly doped systems is valid at least at low temperatures.³

This semiclassical work ignores quantum fluctuations. However, as shown by Reiter,⁵³ for an infinite lattice when quantum fluctuations are included in such variational wave functions one still finds the Shraiman-Siggia dipolar quasiparticles with the long-ranged dipolar spin distortion intact. We have found⁵⁴ that within this lowest-order self-consistent approximation⁵³ the $(\pi, 0)$ states still only involve short-ranged spin distortions, the same as the semiclassical prediction. Thus, it is not unexpected that our quantum cluster and semiclassical analyses agree.

Now let us consider the effect of the short-ranged spin distortions that this kind of quasiparticle produces; viz., why do these quasiparticles not introduce any incommensurate correlations into the spin texture? Given the short-ranged nature of the spin distortion, it is clear that they could lead to a disturbance of the spin texture similar to that found in the quantum dilution problem,¹² since static vacancies also produce a short-ranged disturbance of the spin texture. However, the quantum dilution problem begins with the assumption that the dilutants are randomly distributed throughout a plane. We now show that this is probably not the case for the mobile carriers in the electron-doped materials.

In Ref. 18 we presented some numerics for the hole-hole correlation function for a pair of holes doped into a $\sqrt{8} \times \sqrt{32}$ cluster described by the t - J model. We found that the holes tended to stay as far apart as possible. (It is interesting to note that this is entirely consistent with experimental work purporting to see charge-rich walls, separated by distances scaling like $1/x$, arising from finite-size striped magnetic domains at low x .⁵⁵ Thus, our work demonstrates a magnetic mechanism for such stripes, and is different than the Coulomb-interaction-

generated carrier-rich walls of Emery and Kivelson's³⁴ phase separation ideas.) Since this numerical result is in direct contradiction to the results of Poilblanc,⁵⁶ who studied pairs of holes in a variety of square clusters, we have further scrutinized this behavior. We have found that in (i) Monte Carlo simulations of the t - U model, for an average of two holes in an 8×8 lattice, the holes still tend to want to be as far apart as possible, and (ii) the same behavior is found for the larger $\sqrt{18} \times \sqrt{32}$ 24-site cluster with two holes — these results will be published in a future comment.⁵⁷

We now present our results for similar calculations for the electron-doped system. Figure 6 shows the carrier-carrier correlation function, defined analogously to the hole-hole correlation function of Eq. (6.1) of Ref. 18, by

$$P_{cc}(|i-j|) = \frac{1}{N_T N_e} \sum_{i,j} \left\langle \left(1 - \sum_{\sigma} n_{i,\sigma} \right) \left(1 - \sum_{\sigma} n_{j,\sigma} \right) \right\rangle, \quad (4.1)$$

where $n_{i,\sigma}$ is the hole number operator for electron-doped systems [electron number operator for hole-doped systems, as in Eq. (6.1) of Ref. 18] for spin σ at site i , N_T being the number of lattice sites, and N_e is the number of equivalent sites a distance $|i-j|$ from site i (note that we do not include the angular dependence which is actually present for our nonsquare lattice, for simplicity only,

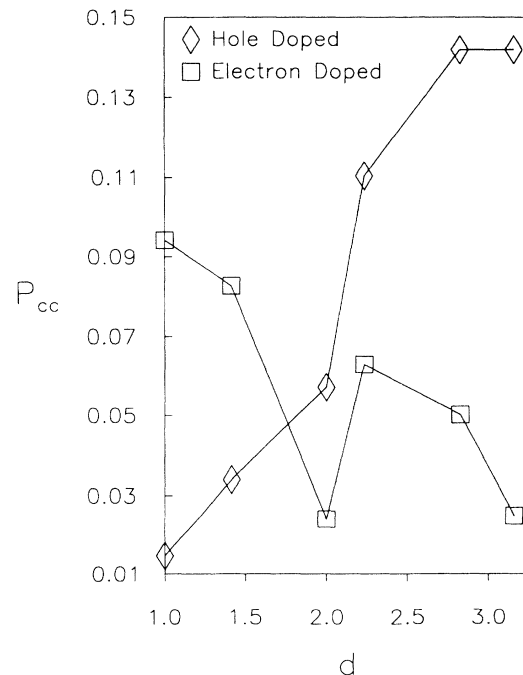


FIG. 6. The carrier-carrier correlation function, defined and described in Eq. (6.1) of Ref. 18, for the hole- ($t' = -0.3$) and electron- ($t' = +0.3$) doped systems, evaluated for the doubly doped state. It is seen that the holes tend to stay as far apart as possible, whereas the mobile electrons tend to cluster together at short distances.

since we have found that this does not affect our conclusions). We evaluated this function for two carriers doped into a $\sqrt{8} \times \sqrt{32}$ cluster described by the t - t' - J model with $t = -1$, $J = 0.4$, and $t' = +0.3$. Juxtaposed with this curve is the analogous hole-hole correlation function for $t = 1$, $J = 0.4$, and $t' = -0.3$. The differences between the two different systems are striking: Whereas pairs of holes tend to stay as far apart as possible, pairs of mobile electrons in the electron-doped system tend to cluster together.

To further elucidate this behavior we have calculated the two-, three-, and four-carrier interaction energies (analogous to the binding energy) defined relative to *independent* carriers (denoted by E_{2I} , E_{3I} , and E_{4I} , where E_n denotes the ground state for n carriers), via

$$\begin{aligned} E_2 &= E_0 + 2(E_1 - E_0) + E_{2I}, \\ E_3 &= E_0 + 3(E_1 - E_0) + E_{3I}, \\ E_4 &= E_0 + 4(E_1 - E_0) + E_{4I}, \end{aligned} \quad (4.2)$$

and our results for both hole- and electron-doped systems are presented in Table II. One sees that for the hole-doped system, the tendency for holes to cluster together is very small — this is consistent with the binding energy study of Riera and Young⁵⁸ (if one uses their definition for the binding energy one finds results very similar to those of Table II). However, for the electron-doped material one finds that there is both a stronger binding of a single pair of holes, as well as a very low interaction energy, at least relative to the hole-doped material, as the number of carriers increases. This shows that the mobile electrons have a much greater propensity to cluster together than do the mobile holes.

Summarizing the numerical work of the last two sections: (i) The single-hole quasiparticles of the hole-doped system are Shraiman-Siggia dipolar quasiparticles. They tend to remain far from each other, and are thus consistent with some form of superposition of these many-body quantum states in the low-doping limit.¹⁸ (ii) The single-carrier ground state of the electron-doped material is different than that of the hole-doped system; viz., it is a $(\pi, 0)$ state as opposed to a $(\frac{\pi}{2}, \frac{\pi}{2})$ state, and a nonzero density of the former tends to exhibit a much stronger tendency to cluster together than do the holes of the hole-doped material. The spin distortions for these quasiparticles are long (short) ranged for the hole- (electron-) doped systems.

TABLE II. Interaction energies, defined in Eq. (4.1), for two, three, and four carriers in the t - t' - J model, using representative material parameters for the hole- and electron-doped compounds based on Eq. (2.4). As long as the single-hole ground states are those that we predict for the hole- and electron-doped systems, these interaction energies do not sensitively depend on the ratio of $|t'/t|$.

	Hole doped $t = 1, t' = -0.3$	Electron doped $t = -1, t' = +0.3$
E_{2I}	-0.12	-0.21
E_{3I}	+0.45	+0.12
E_{4I}	+1.5	+0.26

Considering the data contained in Fig. 6 and Table II, we have reason to believe that for the electron-doped materials the carriers have a strong tendency towards phase separation — certainly the tendency is much stronger than in the hole-doped system. However, since Table II shows that there are not purely attractive interactions between the mobile electron carriers, this tendency will probably lead to the presence of low-energy excited states corresponding to fluctuations into a locally phase-separated state. Then, perhaps these phase-separated states are the cause of the midgap states seen in the photoemission work,²⁶ as was suggested elsewhere.³⁴

As espoused by Emery and Kivelson,³⁴ phase separation in the large hopping limit is likely to be frustrated, the frustration being due to the presence of long-ranged Coulomb interactions. We have investigated the effect of including a near-neighbor Coulomb repulsion between carriers on neighboring sites, and find that no qualitative changes take place until very large Coulomb interactions (say of order much larger than t) are present. However, we do not know how long-ranged Coulomb interactions will affect our conclusions, and this is presently being studied. Further, Trugman⁴¹ noted that tendencies towards the binding of a pair of holes can be greatly reduced by next-nearest-neighbor three-site spin-dependent hopping. While this form of hopping will be of much lower order than the next-nearest-neighbor hopping that we are studying [since we begin with a three-band, not a one-band (as does Trugman), description], and thus we do not expect any qualitative changes in our analysis, we feel it appropriate to see in what quantitative ways our observed tendency towards a phase separated state in electron-doped planes changes with such a hopping term present. Thus, we are also presently studying the effects of such terms.

Consequently, we propose that the commensurate antiferromagnetic spin background of the electron-doped materials do not have incommensurate correlations introduced into them because (i) the quasiparticles introduced into the weakly doped planes are not Shraiman-Siggia dipolar quasiparticles, and (ii) the mobile electrons found in these materials exhibit a form of phase separation, and no incommensurate correlations are expected for such a state of matter. We have completed a study of the electron-hole momentum distribution functions, similar to those presented in Ref. 18, including an evaluation of the density of states for both the hole- and electron-doped compounds, and this work (to be presented later) further strengthens our assertion that some form of carrier clustering is taking place in the electron-doped materials.

V. DISCUSSION

Our numerical results and semiclassical studies have led to the proposal that the single-hole ground states in the hole- and electron-doped materials are different, and that this has a profound effect on (i) their magnetic phase diagrams, and (ii) the tendency towards phase separation that these carriers display. The Shraiman-Siggia

dipolar quasiparticle picture has been shown^{28,29,31,52} to be consistent with many different experiments studying the hole-doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ system, and it will be interesting to see if our $(\pi, 0)$ quasiparticle picture of phase separation in the $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ can be used to explain more than just the ARPES results associated with the midgap states found in ARPES studies.²⁶

One other experiment that may possibly find an explanation in the frustrated phase separation scenario for the electron-doped material involves the resistivity vs temperature results of Hikada and Suzuki.³³ To be specific, if the mobile electrons tend to cluster together for sufficiently long periods of time, the dominant interaction between carriers is electronic as opposed to magnetic, and thus a Fermi-liquid-like $\rho \sim T^2$ is not that surprising. Such a qualitative explanation requires rigorous calculations to be carried out before it is to be taken seriously, and standard transport theories⁵⁹ are available for such studies.

We have addressed the magnetic and other material characteristics of the two 214 high- T_c systems. However, the approach of utilizing the t - t' - J system does not seem to be limited to these single-layer high- T_c materials. Recently, it has been proposed⁶⁰ that hole pockets appear in the $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$ material as one dopes away from the antiferromagnetic insulator, and that these pockets are centered at $(\frac{\pi}{2}, \frac{\pi}{2})$. This is entirely consistent with the "small Fermi surface" observed in ARPES studies of $\text{YBa}_2\text{Cu}_3\text{O}_{6.3}$.⁶¹ In order to model such a system one must include a t' parameter that rotates the Fermi surface by 45° with respect to that predicted by the t - J

model, and to this end we have used $t = 1$, $t' \sim -0.5$, and $J = 0.4$. Then, we find (i) that instead the single-hole ground state occurs at $\mathbf{k} = (\pi, \pi)$ (this was also found in the study of Ref. 44), and (ii) that pairs of such holes tend to stay as far apart as possible, with a hole-hole correlation function similar to that shown for the hole-doped material in Fig. 6. Thus, weakly interacting quasiparticles forming small hole pockets at (π, π) is consistent with our numerics, and are not expected to lead to any incommensurabilities.⁶⁰ Noting that both our semiclassical work (similar to that shown in Fig. 5) and the spin-wave analysis of Reiter⁵³ predict that the spin distortions produced by (π, π) quasiparticles are long ranged, it is very interesting that in the two systems in which the holes tend to stay as far apart as possible the single-carrier quasiparticles produce long-ranged spin distortions, and we are presently exploring this coincidence.

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- Then, the question is, since the holes and electrons both distribute themselves around Sr or Ce defects, why is the spin distortion produced by these systems different? Neither the frustrated-bond (Ref. 8) nor the quantum dilution (Ref. 12) models possess this symmetry. We have found an explanation of this problem, based on our earlier work on this problem, viz., R.J. Gooding, Phys. Rev. Lett. **66**, 2266 (1991), and the details of this will be presented elsewhere.
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