Circulating-current states and ring-exchange interactions in cuprates

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We consider the consequences for circulating-current states of a cyclic, four-spin, “ring-exchange” interaction of the type shown recently to be significant in cuprate systems. The real-space Hartree-Fock approach is used to establish the existence of charge-current and spin-current phases in a generalized Hubbard model for the CuO$_2$ planes in cuprates. We augment the Hartree-Fock approximation to consider correlated states renormalized by Gutzwiller projection factors, which allow us to gauge the qualitative effects of projection to no double occupancy in the limit of strong on-site Coulomb repulsion. We find that charge flux states may be competitive in the underdoped and optimally doped regime in cuprate systems, whereas spin flux states are suppressed in the strongly correlated regime. We then include the ring-exchange interaction and demonstrate its effect on current-carrying states both at and away from half-filling.

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I. INTRODUCTION

The possibility of phases supporting circulating currents in two-dimensional (2D) systems has been debated for some time. The orbital antiferromagnet, or charge flux (CF) phase, was first identified in the context of excitonic semiconductors$^1$ and reintroduced very early in the analysis of high-temperature superconductors,$^{2,3}$ while the spin flux (SF) phase was introduced within a general planar model for the latter.$^4$ On a square lattice, the CF phase [Fig. 1(a)], has counter-rotating currents of carriers on neighboring plaquettes, whence the alternative terminology “staggered flux” phase, and preserves SU(2) spin symmetry but breaks time-reversal invariance. The SF phase [Fig. 1(b)], which can be said to be a fermionic realization of a spin nematic, may be considered as superimposed counter-rotating current patterns in which up- and down-spin currents are equal and opposite (no net charge transport), and preserves time-reversal invariance but violates SU(2) spin symmetry.

A considerable body of theoretical work now exists concerning these states, particularly the CF phase. Early analyses employed the Heisenberg-Hubbard model with an SU(N) generalization of the spin in order to obtain a contolred mean-field decoupling,$^{2,3}$ while further studies have since been performed of the different saddle points obtainable in the $t$-$J$ model.$^5$ The relationship of the CF phase to the superconducting one has been explored in detail within an SU(2)-symmetric slave-boson gauge theory of the $t$-$J$ model by Lee and coworkers,$^6$ and by using a Hubbard X-operator formulation.$^7$ More general models for the cuprate planes, including not only a finite on-site Hubbard interaction ($U$), but also explicit nearest-neighbor superexchange ($J$) and Coulomb interaction ($V$) terms, have been considered using weak-coupling techniques. At half-filling and for $U > 0$, the Hartree-Fock approximation$^4$ (HFA) and more sophisticated renormalization-group analyses of divergent susceptibilities$^8,9$ agree on a phase diagram with magnetic order for weak $J$ and $V$, a charge-density-wave (CDW) phase for strong $V > 0$, CF for $V > 0$ and sufficiently large $J > 0$, and SF for $V > 0$ and $J < 0$. Negative $V$ (nearest-neighbor attraction) yields superconducting phases of singlet symmetry if $J > 0$ and triplet symmetry if $J < 0$.$^{10}$

Interest in the CF phase has been revived recently by an accumulation of experimental evidence suggesting the presence of a quantum critical point in the superconducting region of the phase diagram.$^{11}$ One of the proposals for the “hidden” order parameter associated with the transition is the conventional CF phase, also known as the $d$–density–wave (DDW) state,$^{12}$ although more complex current patterns based on a three-band description have also been proposed.$^{13}$ To date the only experimental means of identifying a CF state is the breaking of time-reversal symmetry, and the interpretation of one such measurement using polarized angle-resolved photoemission spectroscopy$^{14}$ remains open. Circulating-current phases have been considered numerically in the context

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Schematic representation of (a) charge-flux (CF), and (b) spin-flux (SF) phases. Solid arrows represent currents of spin-up electrons and open arrows spin-down electrons.}
\end{figure}
of exact diagonalization (ED) studies of chiral fluctuations in the 2D $t$-$J$ model,\cite{15} and fluctuating staggered currents on a doped ladder,\cite{16} while a more general model displaying steady currents was considered by density-matrix renormalization-group (DMRG) studies in a ladder geometry.\cite{17}

The possible significance of cyclic four-spin, or “ring-exchange”, interactions in cuprates was also recognized at an early stage.\cite{18} The important term arises at fourth order in a strong-coupling (small $t/U$) perturbative expansion of the single-band Hubbard model,\cite{19} and has been shown in this limit to give the leading correction to the nearest-neighbor Heisenberg model. Experimentally, inelastic neutron scattering measurements of the spin-wave spectrum in the 2D system La$_2$CuO$_4$,\cite{20} and in the quasi-one-dimensional spin-ladder compound La$_8$Cu$_8$O$_{11}$,\cite{21} as well as two-magnon Raman scattering measurements on doped systems related to the latter,\cite{22} indicate the presence of ring-exchange contributions. The magnitude of this interaction has been quantified as being 20% of the nearest-neighbor superexchange interaction, i.e. $K \approx J/5$, both by systematic expansion of the three-band Hubbard model,\cite{23} and by a self-consistent spin-wave analysis yielding good quantitative agreement with the experimental data.\cite{24}

At the qualitative level, the presence of a ring-exchange term has been found by consideration of exactly soluble extended Heisenberg models to generate a rich variety of novel phases on a 1D spin ladder.\cite{25} A number of these phases have been found and characterized by ED and DMRG studies of the isotropic ladder.\cite{26} However, for 2D systems accurate results beyond the Hartree-Fock analysis of static magnetic phases\cite{18} remain scarce, and the only numerical study to date was performed for a system with XY spin interactions.\cite{27}

The ring-exchange interaction on a square lattice may be considered as the product of a virtual hopping process around an elementary plaquette, while the CF and SF phases are those in which real currents circulate on the plaquettes. However, to our knowledge there have been rather few studies of the mutual effects of flux states and ring exchange. The issue has been addressed for the CF phase of a $t$-$J$ model with unprojected nearest- and next-neighbor hopping by applying a large-$N$ approach.\cite{28} This study suggested that a ring-exchange interaction acts to suppress the homogeneous CF phase, but may favor inhomogeneous current patterns and other states involving a further breaking of translational symmetry.\cite{27}

Here we adopt a qualitative approach to gain further physical insight into both the real-space nature of circulating-current phases on the 2D square lattice and the influence upon them of ring-exchange interactions. In Sec. II we present the generalized Hubbard Hamiltonian supporting flux phases in the weak-coupling limit and discuss its treatment in the HFA. Sec. III contains a summary of the properties of the CF and SF phases obtained in HFA with unprojected hopping. We turn in Sec. IV to a study of electronic correlation effects, which are included within the Gutzwiller approximation through projected hopping terms, and this allows us to make contact with the physical parameter regime for cuprate systems. In Sec. V we include the ring-exchange interaction and demonstrate its effects on both CF and SF phases at different fillings by analyzing the plaquette current and the ring-exchange energy contribution. Sec. VI contains a summary and conclusions.

## II. MODEL AND FORMALISM

### A. Extended Formalism

To establish the existence of CF and SF phases (Fig. 1) in a 2D lattice we consider the extended Hubbard model in the form

$$\mathcal{H} = H_t + H_U + H_J + H_V + H_K, \quad (1)$$

where the first two terms

$$H_t = -t \sum_{\langle i,j \rangle \sigma}(c^\dagger_{i\sigma}c_{j\sigma} + H.c.) - t' \sum_{\langle i,j \rangle \sigma}(c^\dagger_{i\sigma}c_{j\sigma} + H.c.), \quad (2)$$

constitute the conventional Hubbard Hamiltonian for a single, nondegenerate band with nearest- and next-neighbor hopping. Here $c^\dagger_{i\sigma}$ denotes the electron creation operator, $n_{i\sigma} = c^\dagger_{i\sigma}c_{i\sigma}$, $n_i = \sum_\sigma n_{i\sigma}$, and the notation $\langle i,j \rangle (\langle \langle i,j \rangle \rangle)$ indicates a pair of (next-)nearest-neighbor sites. We adopt $t = 1$ as the unit of energy. The terms

$$H_J + H_V = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + V \sum_{\langle i,j \rangle, \sigma \sigma'} n_{i\sigma} n_{j\sigma'}, \quad (3)$$

correspond, respectively, to superexchange and Coulomb interaction between nearest neighbors. The $t$-$U$-$J$-$V$ model (1) has been considered by a number of authors, including a Hartree-Fock treatment of the infinite system with only nearest-neighbor hopping\cite{29} and RG studies of both the half-filled case\cite{30} with $t' = 0$ and the model with small $t'$ near the van Hove fillings.\cite{31}

Finally, the ring-exchange term in Eq. (1) takes the form

$$H_K = K \sum_{\Box} \left[ (\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{S}_k \cdot \mathbf{S}_l) + (\mathbf{S}_i \cdot \mathbf{S}_l)(\mathbf{S}_j \cdot \mathbf{S}_k) - (\mathbf{S}_i \cdot \mathbf{S}_k)(\mathbf{S}_j \cdot \mathbf{S}_l) \right], \quad (4)$$

where $\Box$ denotes the sum over the four spins $(ijkl)$ of each plaquette labeled clockwise. The phase diagram of a 2D system in the presence of this term has been considered only for the Heisenberg antiferromagnet,\cite{32} although further progress has been possible for 1D magnetic systems.\cite{25,26}
The HFA is the simplest and the most efficient approach for the study of interacting electron systems. Although its application may seem inherently limited to the regime of weak interactions, it provides satisfactory results at all interaction strengths when the correlation energy is small (for example in magnetically polarized phases), and thus can be used to obtain meaningful qualitative insight into the nature of possible ordered phases also for large $U$. In the HFA, multiparticle interaction terms are decoupled into all possible operator pairs, all but one of which are replaced by $c$-number expectation values to leave a single-particle Hamiltonian. In the present analysis the choice of operator pairs with $c$-number expectation values is as follows. Because our primary interest is the study of flux phases, we will work with a repulsive intersite Coulomb interaction $V > 0$, in which case no pairing decouplings need be considered, $\langle c_i^\dagger c_j^\dagger c_j c_i \rangle = 0 = \langle c_i^\dagger c_j c_j^\dagger c_i \rangle$. In the absence of single-site spin-flip terms in the Hamiltonian [Eq. (1)], there is no reason to expect finite averages of the form $\langle c_i^\dagger c_j \rangle$, where $\bar{\sigma}$ denotes the spin projection opposite to $\sigma$. Thus flux phases will compete or coexist with magnetic and possibly charge-ordered phases, and the finite expectation values to be considered are the site charge

$$n_i = \langle c_i^\dagger c_i \rangle + \langle c_i^\dagger \bar{c}_i \rangle,$$

(5)

the site magnetic moment

$$m_i = \langle \mathbf{S}_i \rangle = \frac{1}{2} \sum_{\alpha, \beta=\uparrow, \downarrow} \langle c_i^\dagger \bar{\sigma}_{\alpha \beta} c_{i\beta} \rangle,$$

(6)

and the bond order parameters

$$s_{ij\sigma} = \langle c_i^{\dagger} c_{j\sigma} \rangle.$$

(7)

In a circulating–current state, the latter parameters are complex, $s_{ij\sigma} = |s_{ij\sigma}| e^{i\phi_{ij\sigma}}$, with the real part corresponding to the bond kinetic energy and the imaginary part to the bond current.

For later reference we present the Hartree-Fock decoupling expressions for all of the interaction terms in Eq. (1) in the form in which they will be used here. The Hubbard term is approximated by

$$H_U \simeq U \sum_i \left[ \langle n_{i\uparrow} \rangle n_{i\downarrow} + n_{i\downarrow} \langle n_{i\uparrow} \rangle - \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle \right] + \sum_{i,j} \left[ \langle c_i^\dagger c_j^\dagger c_j c_i \rangle + \langle c_i^\dagger c_j c_j^\dagger c_i^\dagger \rangle - \langle c_i^\dagger c_j \rangle \langle c_j^\dagger c_i \rangle - \langle c_i^\dagger c_j^\dagger c_j c_i \rangle - \langle c_i^\dagger c_i^\dagger c_j c_j \rangle + \langle c_i^\dagger c_i^\dagger c_i c_i \rangle - \langle c_i^\dagger c_i \rangle \langle c_i^\dagger c_i \rangle \right],$$

(8)

where the signs follow from fermionic statistics. We define the effective bond order parameter

$$g_{ij\sigma} \equiv s_{ij\sigma} + \frac{1}{2} s_{ij\bar{\sigma}},$$

(9)
in terms of which a decomposition of the $J$, $V$, and $K$ interactions gives the following one-body terms in the Hamiltonian matrix. For the superexchange interaction

$$H_J \simeq -\frac{1}{2} J \sum_{(ij)\sigma} \left( g_{ij\sigma} c_i^\dagger c_j^\dagger c_j c_i + g_{ij\bar{\sigma}} c_i^\dagger c_j c_j^\dagger c_i \right) + \frac{1}{2} J \sum_{(ij)\sigma} \left( \lambda_{ij} s_i^\dagger s_j^\dagger c_j c_i + \lambda_{ij} s_j^\dagger s_i^\dagger c_i c_j \right) + \frac{1}{2} J \sum_{(ij)\sigma} \left( (S_i^z - i\lambda_{ij} \lambda_{ij} S_j^y) c_j c_i + (S_j^z - i\lambda_{ij} \lambda_{ij} S_i^y) c_i c_j \right),$$

(10)

where $\lambda_i = 1$, $\lambda_i = -1$, and $\{g_{ij\sigma}, g_{ij\bar{\sigma}}\}$ are complex quantities. For the nearest-neighbor Coulomb interaction

$$H_V \simeq V \sum_{(ij)\sigma} \left( n_i c_i^\dagger c_{j\sigma} + n_j c_j^\dagger c_{i\sigma} \right) - V \sum_{(ij)\sigma} \left( s_{ij\sigma} c_i^\dagger c_{j\sigma} + s_{ij\sigma} c_j^\dagger c_{i\sigma} \right).$$

(11)

Finally, the ring-exchange interaction is decoupled into single-particle terms multiplied by all possible combinations of the averages obtained by contracting the remaining six operators,

$$H_K \simeq -\frac{1}{2} K \sum_{(ij)\sigma} \left[ g_{ij\sigma} c_i^\dagger c_j c_i + g_{ij\bar{\sigma}} c_j^\dagger c_j + \lambda_{ij} c_i^\dagger c_j c_i \right] \sum_{(kl)(ij)} \left( \langle \mathbf{S}_k \cdot \mathbf{S}_l \rangle \right) + \frac{1}{2} K \sum_{i,j(i)\sigma} \left[ (S_i^z - i\lambda_{ij} \lambda_{ij} S_j^y) c_i c_i + \lambda_{ij} S_j^z c_i^\dagger c_i \right] \right) \times \sum_{(kl)(ij)} \left( \langle \mathbf{S}_k \cdot \mathbf{S}_l \rangle \right),$$

(12)

with the intersite spin correlation function, determined within HFA, given by

$$\langle \mathbf{S}_k \cdot \mathbf{S}_l \rangle = \langle \mathbf{S}_k \rangle \langle \mathbf{S}_l \rangle - \frac{1}{2} \left( s_{kl\uparrow} s_{kl\downarrow} + s_{kl\downarrow} s_{kl\uparrow} \right) - \frac{1}{2} \left( |s_{kl\uparrow}|^2 + |s_{kl\downarrow}|^2 \right).$$

(13)

The structure of the decomposition is similar to that of the superexchange term, although in this case the net contributions are quartic in $\langle \mathbf{S}_i \rangle$ and $\langle c_i^\dagger c_j \rangle$, so may be expected to be small at the Hartree-Fock level. Note that in Eqs. (10-12) we have omitted the constant terms bilinear in the expectation values [analogous to the final term in each line of Eq. (8)].

C. Self-consistent calculations in real space

We have performed calculations on a finite cluster in real space to establish the microscopic conditions under which the CF and SF phases are manifest as circulating currents of real electrons (or holes), which arise from a mismatch in hopping expectation values between the two directions along each bond in a coherent pattern. These bond expectation values, the site charges, and the site magnetic moments are computed for any set of interaction parameters and iterated to self-consistency. The
HFA in real space has been used extensively for qualitative modeling of cuprate systems, and in particular for the analysis of charge-inhomogeneous stripe and other density-wave phases, which it tends to favor. A full review of the technique is presented in Ref. 29, and we summarize here those aspects of its application which are important for the current analysis.

Most importantly, the HFA suppresses fluctuation terms and thus favors (homogeneous or inhomogeneous) ordered states which minimize static interactions. Magnetic and charge-density interactions, which are zeroth-order in particle-hopping fluctuations, are enhanced relative to kinetic terms, and it is for this reason that the method tends to find ground states with inhomogeneous charge distributions and/or magnetic order. By contrast, methods such as the Hubbard X-operator and other large-\(N\) approaches have a tendency to favor kinetic terms, as a result of which they do not show stripe phases and often produce flux-phase ground states. Thus a real-space Hartree-Fock analysis is not an appropriate framework for an unbiased discussion of energetic contributions and true ground states; in specific terms, the flux phases we investigate are frequently local rather than global energy minima. Mindful of this fact, we will restrict our considerations to qualitative statements concerning the nature of circulating-current phases and the relative effect upon them both of doping and of the different interactions, particularly the ring-exchange term.

We note also that the method is especially sensitive to the choice of starting state, as well as to boundary conditions and in some cases to commensurability effects due to the electron filling. A careful specification of these extrinsic variables is required in order to make meaningful comparisons yielding intrinsic electronic properties.\(^{29}\) We will consider a system of size \(N = 12 \times 12\) sites with periodic boundary conditions; qualitatively similar results were obtained with systems of size \(8 \times 8\) and \(16 \times 16\), and we have established that flux states may be found for any rectangular system with even-length sides. Open boundary conditions lead to a suppression of circulating currents and to inhomogeneous edge values, and are not considered further. The establishment of global, as opposed to local, energy minima may be pursued as in Ref. 29, but for comparative studies of flux states is not of prime importance (preceding paragraph). Finally, by considering the evolution of the results with electron filling we will demonstrate that commensuration effects are absent and thus that the system size is sufficient for robust qualitative conclusions.

III. CIRCULATING-CURRENT STATES

A. Dependence on doping

We begin by establishing homogeneous flux phases in the generalized Hubbard model on a cluster. As expected from the weak-coupling results mentioned in Sec. I,\(^4,8,9\) we find that the nearest-neighbor interactions \(J\) and \(V\) are of crucial importance: circulating-current states appear close to half-filling only for simultaneously large values \((>1)\) of the interaction ratios \(|J/U\) and \(4V/U|\). The CF phase, with finite currents of up- and down-spin electrons moving in the same direction [Fig. 1(a)], occurs when \(J > 0\) and SF states, with counterflowing up- and down-spin currents, appear for \(J < 0\). The parameter sets for flux-phase formation are dictated by the strong propensity within the real-space Hartree-Fock approach towards charge localization, driven by large values of \(U\), charge inhomogeneity driven by large \(V\), and phase separation driven by large \(J\). In this section we characterize the dependence of the homogeneous CF and SF phases on the doping and on the magnitude of the interactions.

We define the filling as the normalized number of electrons in the system, \(n = N_e/N\), and the hole doping as \(x = 1 - n\). We choose the parameters \(U = |J| = 4V = 4t\), and show in Fig. 2 the doping dependence of the bond order parameter [Eq. (7)] for a single spin species and a single direction along an \(x\)- or a \(y\)-axis bond. The real part \(T = \text{Re} s_{ij}\) is a component of the bond kinetic energy, and constitutes one eighth of the hopping kinetic energy per site of the system, while the imaginary part \(I = \text{Im} s_{ij}\) corresponds to one half of the bond current for a single spin species (and thus to one quarter of the charge current in a CF phase). It is clear that, for moderate interaction strengths, circulating-current states are robust close to half-filling. However, the current shows a monotonic decrease as a function of doping until the CF and SF phases become unstable at doping values of 0.16-0.18.

The magnitudes of the (negative) real parts \(T_{\text{CF}}\) and \(T_{\text{SF}}\) are scarcely affected by the presence of the currents. In the absence of flux phases or other types of order, \(T\) is expected to be constant at low doping for the cluster under consideration, beginning to drop beyond \(x = 0.153\); this number does not affect the behavior of established ordered phases. For the intermediate coupling strengths

FIG. 2: Doping-dependence of kinetic energy per bond for each spin orientation as obtained in HFA for CF \((J > 0)\) and SF \((J < 0)\) phases with \(U = |J| = 4V = 4t\).
the fact that the current “order parameter”, $I$, the interaction ratios as functions of interaction strength for a fixed choice of with competing phases allowed by these symmetries. This contrasting behavior may be taken as a reflection of the different symmetries broken by the two phases (Sec. I), through the coexistence with competing phases allowed by these symmetries.

B. Dependence on interaction strength

The CF and SF states for small doping are characterized in Fig. 3(a), which shows the quantities $T$ and $I$ as functions of interaction strength for a fixed choice of the interaction ratios $|J|/U = 4V/U = 1$. Qualitatively, the current does not contribute to the overall kinetic energy, and the finite imaginary part of the bond hopping parameter is stabilized by Fock terms originating from decouplings of the $J$ and $V$ interactions, as seen in the presence of the negative signs in the first line of Eq. (10) and the second line of Eq. (11). Figure 3(b) compares the kinetic energy contribution to the total energy, illustrating the dominance of the static, zeroth-order interaction terms contained in Eqs. (10) and (11). While the kinetic contribution remains nearly constant, the total energy increases monotonically, reflecting the penalty for failure to adopt charge- or magnetically ordered states. It is this failure which ultimately destabilizes the CF and SF phases, rendering them uncompetitive in comparative HFA studies in real space.

One observes again that growth of the current has little effect on $T_{\text{CF}}$ in Fig. 3(a), and that $I_{\text{CF}}$ saturates with increasing interaction strength, approaching the limit $|T_{\text{CF}}| = |I_{\text{CF}}|$ where the phase per bond is $\chi_{ij} = \pi/4$. Thus the phase $\phi$ for a plaquette approaches $\phi = \pi$, and the CF state is the $\pi$-flux phase of Ref. 2. By contrast, in the SF state $I_{\text{SF}}$ continues to rise with increasing interaction strength, the kinetic contribution $T_{\text{SF}}$ falls, and this phase becomes unstable to a symmetry-broken magnetic state with finite net moment. We note also that the flux states remain stable in the limit of vanishing interactions, although in this case they are not the global energy minima of the system. A similar situation is found by analysis of different saddle points in a large-$N$ approach: for the SU($N$) saddle point, which yields the CF state, the circulating-current phase also survives at zero interaction strength. While Fig. 3 illustrates the situation for $x = 0.028$ (4 holes in a $12\times12$ system), the same behavior is found at higher doping: for $x \approx 0.1$ the evolution of the bond phase in the SF state is almost identical, while for the CF state it converges more slowly to $\pi/4$, and the current in the zero-interaction limit is somewhat smaller.

C. Dependence on next-neighbor hopping

The effect of a next-neighbor, cross-plaquette hopping $t'$ in Eq. (2) is shown in Fig. 4. We have computed the bond-order parameters for both nearest- and next-nearest-neighbor bonds for charge- and spin-flux phases over the range of values of $t'$ for which these phases are maintained. The qualitative behavior is the same for all dopings in Fig. 2, and is illustrated for an intermediate choice of $x$. We have defined $t$ and $t'$ with inclusion of a negative sign in Eq. (2), so $t = 1$ and $t' < 0$ corresponds to the physical sign for cuprates. We note also that for clarity of presentation Fig. 4 shows $|T| = -T$ but the true sign of $T'$. The most interesting feature is that small values of $t'$ have no effect at all on CF and SF states, in that the expectation values of the bond energy and current, which are determined largely by $H_J$ and $H_V$ in Eq. (1), are not changed by the additional kinetic term. In this regime, which persists more strongly for negative $t'$, diagonal hopping gives a very small contribution to the energy which is positive for $t' < 0$. Negative values of $t'$ show a small tendency to reinforce both types of flux phase, by which is meant to increase the bond current with a concomitant small decrease in bond energy, which
in the context of cuprate systems is a noteworthy result. Positive values of $t'$ show a more pronounced tendency to suppress both types of flux phase; for the CF state there is a stable small-current regime over a range of values of $t'$, in which the next-neighbor hopping contribution to the kinetic energy is quite significant.

The regions of stability are cut off for both signs of $t'$ as the need to minimize the total kinetic energy drives transitions to phases with similar energetic contributions from both nearest-neighbor and diagonal bonds. These states are marked by a sharp rise in $|T'|$. For the CF state this process occurs for $|t'| \sim t$, and involves homogeneous zero- or small-current phases. For the SF state the transitions involve inhomogeneous phases of small total kinetic energy and non-zero magnetic moments, and occur for significantly smaller $|t'|$. This latter result may be taken as evidence that the SF phase is generally less stable to competing phases [Fig. 3(b)]. We stress that the values of $t'$ required to destabilize the CF and SF states at this filling should not be considered as quantitatively representative, and emphasize only the qualitative behavior in the presence of $t'$. The results are consistent with the renormalization-group analysis of Ref. 9 for the physical sign of $t'$ ($t' < 0$ in our notation convention), in which the location of the CF phase boundary is scarcely affected for $|t'| < 0.3$, whereas the SF phase is entirely suppressed. Further studies of the role of diagonal hopping, including consideration of circulating-current phases established on the diagonal bonds at very large values of $|t'|/t$, have been conducted in Ref. 28.

We conclude this survey of the qualitative properties of flux phases in the weak-coupling regime by commenting that in the unrestricted Hartee-Fock approach essentially no inhomogeneous current-carrying states were found. While the method presents no barriers to phase coexistence, over most of the parameter range the coexisting flux-phase components are small compared to other, competing phases, and only a very weak, uniform current pattern is maintained. This situation may be altered in the presence of a relatively large next-neighbor hopping parameter $t'$, which also raises the possibility of obtaining specific inhomogeneous current configurations, but this parameter regime is of little physical interest in the context of cuprates, and is not considered here.

IV. FLUX PHASES WITH STRONG CORRELATIONS

A. Gutzwiller Approximation

The analysis of the preceding section is limited to the regime of weak coupling. However, interactions in cuprates are strong, and in particular the large on-site repulsion $U$ causes a suppression of double site occupation due to electronic correlations, which is not taken into account in the unrestricted HFA. As a consequence, the parameter regime in which flux phases were found in Sec. III has little relation to the model parameters appropriate for superconducting cuprates. In this section we use the Gutzwiller Approximation (GA), which includes strong correlations through their effect in suppressing states including doubly occupied sites from the Hilbert space, and thus allows us to approach the cuprate parameter regime. Because the GA reproduces qualitatively the effects of (partially or fully) projected hopping on the single-particle level, an adapted HFA of the type employed in Sec. III remains valid. Recent considerations of Gutzwiller wave functions for multiband models have also led to an improved understanding of the Mott transition in these systems.

While many of the early analyses of flux phases in cuprate-related models employed an effective large-$U$ description such as the $t$-$J$ model, relatively few of these employed the projection of the hopping term associated with the constraint of suppressed double site occupancy. This constraint, which with full projection yields a hopping term of the form

$$H_t = -t \sum_{(i,j)\sigma} \left[ (1-n_{i\sigma}) c_{i\sigma}^\dagger c_{j\sigma} (1-n_{j\bar{\sigma}}) + \text{H.c.} \right]$$
\[- t' \sum_{\langle i,j \rangle \sigma} [(1-n_{i\sigma})c_{i\sigma}^\dagger c_{j\sigma}(1-n_{j\bar{\sigma}}) + \text{H.c.}], \]  

(14)

is technically very difficult to implement systematically. Because of its singular nature the connection between unprojected (independent electron) and projected models remains quite unclear, and the possibility arises that flux phases may indeed be far more relevant for the latter. One exact means of implementing projected hopping is in numerical studies, such as the exact diagonalization analysis of uniform and staggered flux phases in the \(t-J\) model\(^{31}\) and of the CF phase in the presence of hole pairing.\(^{32,33}\)

Here we approximate the projected model by the Gutzwiller approach,\(^{34}\) in which electron correlation effects are contained within multiplicative prefactors modifying the terms of the Hamiltonian. These prefactors are obtained from statistical considerations based on the numbers of states available and excluded by the constraint.\(^{35}\) This approximation to the effects of a large \(U\) term was presented for the 2D Hubbard model in Ref. 36, where the technical details are also summarized. For the purposes of controlling the extent of projection, here we apply these factors in their general form at finite \(U\) (see also Ref. 37)

\[ g_t = \frac{(n-2d)(\sqrt{d} + \sqrt{1-n+d})^2}{n(1-\frac{1}{2}n)}, \]

\[ g_J = \frac{[(n-2d)]^2}{n(1-\frac{1}{2}n)} = g_{11}^{\text{V}}, \]

\[ g_V^{12} = \frac{2d(n-2d)}{n^3(1-\frac{1}{2}n)} \quad g_V^{22} = \frac{16d^2}{n^4}, \]

(15)

where \(g_t, g_J, \) and \(g_V^{mn}\) multiply the corresponding terms in Eq. (1). The variable \(n\) is the electron filling (Sec. III.A), and the parameter \(d\) represents the density of doubly occupied sites in the system, \(d = \langle n_{i\uparrow}n_{i\downarrow}\rangle\). Because we consider only those uniform phases found in the HFA analysis of Sec. III, the density \(d\) is independent of \(i\). For finite values of \(U\), three terms are required to represent the nearest-neighbor Coulomb interaction, depending on the occupation state of the sites involved. Because the number of bonds with at least one doubly and one singly occupied site is low for all parameters and dopings under consideration, it is a very small and thus acceptable approximation to proceed with a single factor \(g_V \equiv g_V^{11}\).

The effective model with projected hopping is considered to be derived from a Hubbard model with large but finite \(U\).\(^{19}\) Thus the parameter \(d\) is nonzero, in accord with the finite values of the \(J\) and \(V\) terms, whose physical origin lies in virtual hopping processes involving an effective double site occupancy. We define the quantity \(d_0(n)\) as the average value of the double site occupancy for a fixed, finite value of \(U\) at each electron filling \(n\), as determined in the HFA to the correlated state \(\langle d_0(n) \rangle < \langle n/2 \rangle^2\) because this reference Hartree-Fock state is magnetic. An effective \(t-J-V\) Hamiltonian with projection factors \(g_t, g_J, \) and \(g_V\) determined using \(d_0(n)\) in Eq. (15) should then represent the starting \(t-U\) Hamiltonian. Within this framework, projection to a lower net double occupancy \(d < d_0(n)\) is a variationally motivated procedure which seeks to minimize the total energy by further elimination of the energetically costly doubly occupied sites, the limit of this process being a full projection with \(d = 0\). In Sec. IV.C we will use \(d\) as a variable parameter to illustrate the interpolation between the unrestricted HFA and the strongly correlated state for the same electron density \(n\). We note, however, that only small corrections to the energy and magnetization are expected due to this procedure in the strongly correlated regime, because the unrestricted HFA already captures most of the relevant effects, and for large \(U\) approaches the same limit as the projected model.\(^{38}\) While this partial projection procedure is of limited meaning in the context of a model with arbitrarily chosen values of \(J\) and \(V\) as in Sec. III, the effective model used in this section is that obtained by large-\(U\) expansion of the Hubbard model (2). The parameters \(J\) and \(V\) in Eq. (1) thus have the specific values \(J = 4t^2/U\) and \(V = -J/4\).

Further insight into the physical meaning of the GA and its relation to the Gutzwiller projection for cuprate systems, may be obtained from the consideration of variational wave functions, a study which has been undertaken both for superconducting states\(^{39}\) and for coexisting superconducting and CF states.\(^{40}\) We note here that the partially projected states used in this framework are not appropriate for addressing the Mott transition at half-filling, as has been shown systematically from their violation of optical sum rules.\(^{41}\) At finite doping these considerations bear a certain similarity to the recent discussion of “gossamer” superconducting states\(^{37,42}\).

For the purposes of analyzing flux phases in a cuprate-relevant model with projected hopping, we begin by considering a Hubbard model with \(U = 12\). The Hartree-Fock density \(d_0(n)\) of doubly occupied sites is then computed for all values of the filling \(0.8 \leq n \leq 1\) \((0 \leq x \leq 0.2)\). An effective projected model is obtained by computing the Gutzwiller factors [Eq. (15)] at each filling by varying \(d\) between the values \(d = 0\), which describes full projection and is implemented to extract the properties of correlated electrons as described by a \(t-J\) model, and \(d = d_0(n)\), which should reproduce qualitatively the unprojected (Hartree-Fock) states. The final version of the effective model is then as in Eq. (1), but with \(t\) replaced by \(g_t\), \(J\) replaced by \(g_J t/3\), \(V\) by \(-g_j t/12\), and no on-site repulsive term. We emphasize that the derivative of this effective model involves a singular truncation rather than a systematic transformation, with the consequence that no meaningful energetic comparisons are possible between the results of Sec. III and the results obtained after projection. However, it is important to understand the general properties of the projected system, and comparisons performed within it remain well defined.
B. Qualitative consequences of Gutzwiller Approximation

Qualitatively, one of the principal effects of projection is to sharpen the competition between the different candidate ground states. The exclusion of doubly occupied states eliminates most of the possibilities for a coexistence of localized and delocalized phases, and phase boundaries would thus be expected to become better defined. For CF phases these boundaries may also move closer to a parameter regime meaningful for cuprates (see below): when viewed as a means for dynamical holes to avoid each other (by circulating around each other on plaquettes), the CF state indeed allows a greater spatial separation than the superconducting state while retaining a favorable kinetic energy. However, application of this schematic picture for the SF phase, which requires in principle that up- and down-spin particles can move past each other on each individual plaquette, suggests that this type of state would be completely suppressed by projection.

By inspection of the Gutzwiller prefactors (15) it is clear that close to half-filling the properties of the projected model are significantly different from those of the unprojected model. With full projection the factor \( g_t \) vanishes as \( x \to 0 \), giving a complete suppression of the kinetic contributions to the total energy, and also of any bond currents. This suppression is large for small doping, where the kinetic and current terms are significantly smaller than in the unprojected system. However, because all competing states are similarly affected by projection, this does not imply that circulating-current states must become less competitive. By contrast, for small \( d \) the prefactor \( g_t \to 4 \) as \( x \to 0 \), suggesting a relatively strong enhancement of magnetic interactions. Once again, because the superexchange interaction has both spin and bond-order decouplings [see Eq. (10)], this trend does not necessarily imply a suppression of flux states. The prefactor \( g_t \) is smaller than \( g_I \), and is not expected to play a significant role. For larger values of \( x \) these statements remain generally true while \( U \) is large, and \( d \) correspondingly small, but the relative strengths of the kinetic and magnetic terms will change almost linearly with \( x \).

C. Partial projection

We begin the more quantitative part of the analysis by considering the evolution of the flux phases with the extent of projection of the hopping term. Following the above discussion we define a partial projection variable

\[
p = d/d_0(n),
\]

such that \( p = 0 \) corresponds to fully projected hopping (14), and \( p = 1 \) to a projection at finite \( U \) which represents (by reference to the average number of doubly occupied sites) the HFA of Sec. III. Fig. 5 shows the bond energy and current of a CF state as a function of \( p \) for a system with 140 electrons \((x = 0.028)\), while this doping illustrates most clearly the effects of projection, qualitatively identical results are found for higher values. At larger values of \( p \), which correspond to relaxation of the constraint and thus to a larger relative kinetic contribution, \(|T_{CF}| \) and \( I_{CF} \) change linearly with \( p \), and have a fixed ratio (corresponding to a plaquette phase \( \phi \sim 2\pi/3 \)) which decreases with increasing doping. As full projection \((p = 0)\) is approached the suppression becomes stronger, and the real and imaginary parts tend to fixed values determined by the filling; their ratio increases with projection up to an equivalent flux \( \phi = 0.88\pi \) for this doping.

The SF phase exists only for negative values of the superexchange \( J \), which is not a valid parameter regime in the framework of a small \((t/U)\) expansion for the Hubbard model. If the sign of \( J \) is simply inverted, the calculation does not converge to a stable local minimum corresponding to a SF state for any partial projection. The projection factors contribute in two ways to this result: the fact that \( I_{SF} \) approaches \(|T_{SF}| \) \((\phi \to \pi)\) reduces a difference term [which for the CF state is a sum, causing the difference visible in Fig. 3(b)] contributing a negative energy, and the suppression of the total kinetic energy removes what is then an essential negative contribution. This failure to form an SF state in the projected real-space HFA, which extends to all values of the doping \( x \), may be taken as evidence that the schematic picture of counter-flowing up- and down-spin currents, which implies that electrons must hop past each other on each site, is in fact a valid description of this phase.

With regard to the total energy of partially projected CF states, the increasing kinetic contribution as projection is relaxed \((p \to 1)\) means that the fully projected state has the highest energy. We have commented in Secs. II and IV.A on the restrictions concerning meaningful energetic comparisons because of both the nature of the HFA and the singular projection scheme. Within the manifold of projected CF states, changes in total energy as a function of \( p \) are dominated by the kinetic energy.

![Fig. 5: Kinetic energy \( T \) and current \( I \) per bond for each spin orientation in a CF state for with partially projected hopping for \( x = 0.028 \) and \( J = -4V = t/3 \).](image-url)
term, and, in the framework of a consistent derivation from the Hubbard model, no systematic study of energies, for example as a function of interaction strength [Fig. 3(b)], is then possible. However, it is clear from our calculations in the projected regime that the energy difference between the CF state and other competing phases, such as antiferromagnetic order, is small.

While we caution as before that quantitative conclusions cannot be drawn, and note also that energy scales are altered by projection, it does appear meaningful to state that, unlike in the unprojected framework, CF phases are strongly competitive in a projected model. This statement applies not only to the most favorable choice of interactions (Sec. III) but specifically for cuprate parameters. The enhanced competitiveness of the CF state indicates that projection provides a better reflection of the energy gained by dynamically stabilized phases, the origin of which lies primarily in bond-order decouplings of the $J$ and $V$ terms. We may conclude from this consideration of the GA that CF phases are not in fact unrealistic for cuprate interactions when appropriate projection of the hopping terms is performed. More quantitative analyses of this issue are required.

### D. Dependence on doping

We consider next the dependence of the fully projected ($p = 0$) CF state on doping. The evolution of the bond parameters $|T_{CF}|$ and $I_{CF}$ with $x$, shown in Fig. 6(a), exhibits three important qualitative features. First, the effective projected model approaches the $\pi$-flux phase, $|T_{CF}| = I_{CF}$, when the doping decreases towards half-filling. However, in this limit the kinetic energy and current also vanish in the projected model, in contrast to the unprojected one. Secondly, the kinetic component increases linearly in magnitude (becomes more negative) with hole doping across the full range of $x$, tending towards the value found for a projected metallic state (not shown). Finally, the bond current grows at first, but beyond $x \sim 0.08$ falls continuously to zero (at $x_c \simeq 0.16$), indicating the instability of the CF state to a metallic (Fermi-liquid) phase at higher doping.

We stress that in the projected model the kinetic terms are no longer identical to the real and imaginary parts of the bond-order parameter $s_{ij}$, but are related by a ratio of Gutzwiller factors (15). The components of $s_{ij}$, which are determined by the bond decoupling of the terms $H_1$ and $H_V$ in Eq. (1), are shown as functions of doping in Fig. 6(b). The absolute value of the bond amplitude $|s_{ij}|$ decreases only slightly with doping, while the bond phase falls continuously from $\pi/4$ at half-filling to zero at $x_c$. At a qualitative level, the monotonically decreasing Im $s_{ij}$ and dome-shaped form of $|I_{CF}|$ are rather similar to the behavior of the pseudogap amplitude and order parameter for $d$-wave superconductivity computed in the projected BCS wavefunction framework in Ref. 39. Given that we have chosen to allow only bond order, but no pairing decouplings, such a similarity may be expected from the SU(2) symmetry relationship of CF and superconducting phases in this class of models.9 The microscopic origin of a coexistence of paired and CF states has been investigated by a number of authors,32,33,43 At the quantitative level, the net hopping kinetic energy per site $|E_t| = 8|T_{CF}|$ in Fig. 6(a) is for all dopings within 15% of the value calculated in Fig. 4(a) of Ref. 40 using a projected wave function approach to the SC phase. This result underlines the energetic similarity of the SC and CF phases, and the need for a detailed and unbiased analysis to distinguish between them.

We discuss only briefly the dependence of the CF phase on the strength of electronic interactions in the extended Hubbard model. Within the framework we have established for the Gutzwiller analysis this means an alteration in the value of $U$, and for increasing $U$ one approaches the asymptotic regime where $d_0(n) \propto (t/U)^2$. However, as $d_0(n)$ becomes smaller than its value for $U \simeq 8$, the Gutzwiller projection factors (15) are governed primarily by the doping $x$. This reflects the fact that increasing doping causes a gradual release of the constraints arising from strong correlations. In the large-$U$ regime of most interest it is thus the filling rather than the double occupancy which is the most important parameter.
determining the current and the bond phase of the CF state.

E. Dependence on next-neighbor hopping

Following the analysis of Sec. III, we consider also the effect of a next-neighbor hopping $t'$ on the fully projected CF phase, shown in Fig. 7. As observed also for the unprojected model (Fig. 4), small values of $t'$ have no effect on the bond-order parameters $T$ and $I$, and the $T'$ contribution, which is positive at $t' < 0$, is essentially a residual consequence of the prevailing CF state. The regime of stability for the projected CF phase extends considerably further for negative than for positive $t'$, with its midpoint at $t' \sim -0.3$: it appears reasonable to state that for the physical magnitude and sign of $t'$ in cuprates, next-neighbor hopping does not disrupt and may in fact reinforce the CF state.

The CF phase is again terminated by abrupt transitions to zero-current states for sufficiently large values of $t'$. For $t' > 0$ a transition occurs at rather small $t'$ to a phase with strongly reduced bond kinetic energy. However, beyond this we find a further CF phase with a small but finite current, which permits a significant $T'$ contribution. This new phase persists to $t'/t > 1$ before being replaced by another state, of zero current, which again has strongly reduced $|T|$ due to manifestly frustrated hopping. For $t' < 0$ the conventional CF phase persists down to $t'/t \sim -1$ before being replaced by a zero-current state which achieves negative kinetic energy on both nearest-neighbor and diagonal bonds, with $|T|$ only slightly suppressed from its value in the CF state.

V. RING-EXCHANGE INTERACTION

We turn next to the effects of the four-spin ring-exchange interaction on the flux states of Secs. III and IV. Because the structure of this term is quadratic in bilinear spin terms (4), the structure of its Hartree-Fock decomposition (12) is similar to that of the superexchange term (10). However, in addition to nearest-neighbor spin and bond expectation values it contains also next-neighbor bond-order terms corresponding to the diagonals of each plaquette. These appear in the Hamiltonian matrix in the same position as next-neighbor ($t'$) hopping terms. The quartic nature of the ring-exchange interaction $K$, and the relatively small expectation values of the order parameters $\langle S_i S_j \rangle \leq 0.25, |s_{ij}| \leq 0.25$, suggest that the effect of this term in an unprojected model will be small for all but the largest values of $K$.

A. Unprojected model

The qualitative influence of the ring-exchange interaction on the unprojected CF and SF phases of Sec. III may be assessed by considering the changes in bond currents, and also the total energy contribution, due to the presence of the four-spin coupling term. Figure 8(a) shows the bond current in a system with a representative intermediate value of doping for a canonical choice of flux-phase interaction ratios $U = |J| = 4V = 4t$ over a range of values $-|J| \leq K \leq |J|$. It is clear that a positive ring-exchange interaction suppresses the CF state, whereas it acts to enhance the current in the SF state.

These qualitative results may be explained by considering the “interference” of currents on opposite bonds of
each plaquette, which are coupled by the $K$ term in the manner shown in the first line of Eq. (12), and specifically from the role in this interference of currents with opposing spins [second term of Eq. (13)]. The suppression of the CF state by a ring-exchange interaction is in agreement with the findings of Ref. 28; enhancement of the SF state is also consistent with a recent exact diagonalization study of a small cluster with $K$ as the dominant interaction, which revealed a type of SF phase. \textsuperscript{45} We comment further on this result below.

The ring-exchange contribution to the total energy, shown in Fig. 8(b), is by its quartic nature always positive for $K > 0$. This energy, $E_K$, constitutes a significantly smaller penalty in the SF state than in the CF state. Examination of the total energy (not shown) reveals a similar increase for the CF state, reinforcing the result of the preceding paragraph. For the SF state the total energy also shows a small increase of the same order as $E_K$, suggesting that changes in the kinetic and magnetic energies induced by the enhanced current do not compensate the positive ring-exchange contribution. As a function of filling, the influence of the $K$ term on the quantities characterizing the flux phases remains as shown in Fig. 8 and displays no strong variation over the range $0 \leq x \leq 0.2$.

We have also computed the bond currents and ring-exchange energies of flux phases with $K = |J|/5$ for the full range of doping values over which these exist. The current differs only very slightly from its values at $K = 0$ (Fig. 2), although there is a slight suppression which brings the CF transition to a lower doping value. The energy $E_K$, which is illustrated in Fig. 9(a), shows only minor changes with increasing $x$ until the transition to a different (non-flux) state brings abrupt alterations at the critical dopings. The relative changes in current and energy are both understood readily from the evolution of $s_{ij}$ in the flux states at $K = 0$ (Sec. III). However, we draw attention of the magnitude of these effects: even for $K = |J|$ these are in the percent range, and for the physical parameters of cuprate systems, $K \sim J/5$, they are quantitatively irrelevant.

### B. Projected model

In Sec. IV we have shown that circulating-current states are significantly more competitive in projected models for strongly correlated electrons than in HFA. On first inspection one may also expect ring-exchange interactions to be considerably more relevant in a projected Hamiltonian: the appropriate Gutzwiller prefactor for the $K$ term is $g_K = g_J^3$, which approaches 16 at half-filling. To examine this possibility, in Fig. 10 we show for an intermediate doping the projected analog of Fig. 8, following the bond current and ring-exchange energy in a fully projected CF state as a function of $K$. Both quantities show the same essentially linear trend which follows...
from suppression of the CF phase in the presence of a positive ring-exchange interaction. With regard to the doping-dependence of $I_{\text{CF}}$ and $E_{K, \text{CF}}$, as in the unprojected case the current is dictated by the $K = 0$ behavior of the system [Fig. 6(a)], with a small reduction in critical doping for positive $K$. The ring-exchange energy for the projected model with $K = J/5$ is shown in Fig. 9(b), and exhibits a steady decline which may be traced to the combination of $s_{ij}$ parameters [Eqs. (12, 13)] as the bond phase decreases from $\pi/4$ to 0 [Fig. 6(b)].

Returning to Fig. 10, in fact the ring-exchange effect on the current in the projected CF phase is significantly larger than in the unprojected one (10% compared to 2% at $K = J$ for $x = 0.083$). This result holds for all dopings, and extends also to the relative magnitude of the energy contribution $E_K$. However, it is clear that changes in both energy and current remain extremely small: this is not surprising given that the energetic contribution of the $K$ term is multiplied by the fourth power of bond expectation values $s_{ij}$ which are suppressed towards zero at half-filling for full projection. In this context we note that ordered magnetic states suffer no such suppression of the order parameter on projection, and thus from the large value of $g_K$ a Gutzwiller-projected model near half-filling might be expected to favor the formation of magnetic phases stabilized by large values of $K$.

C. Phases in the large-$K$ regime

We thus conclude this section by commenting briefly on the effects of a very strong ring-exchange interaction. In spin systems, as realized at half-filling for large $U$, the ring-exchange term is generally considered to favor a maximization of the solid angle of the four spins on a plaquette, and thus to yield non-collinear magnetic phases. In the large-$K$ limit one expects the (static$^{18}$ or dynamic$^{25,26}$) vector-chirality phase depicted in Fig. 11(a). This type of spin configuration has a low bond kinetic energy but a finite spin flux in the sense familiar from double-exchange models,$^{46}$ that a propagating electron picks up a path-dependent phase. In practice the bond current and kinetic energy vanish at half-filling in this static limit for large-$U$ systems. In the presence of holes a strong ring-exchange interaction is also expected (from the magnitude of the expectation values involved) to promote magnetic rather than bond order.

However, in our analysis of the large-$K$ limit for an unprojected model with $U/t \gg 1$, both at and away from half-filling, we have found a different ground state, shown in Fig. 11(b). This spin configuration ensures a “three-up, one-down” state on every plaquette, which gives the same ring-exchange energy per plaquette [see Eq. (4)] as the vector-chirality configuration. It is not unique, and need not conserve a total spin component $S_z^{\text{tot}} = 0$. The extra stability of the “three-up, one-down” phase may be ascribed primarily to the fact that, in approaching the limit of an effective spin model, residual dynamical processes act to favor collinear spin states. However, quantum fluctuations not contained at the Hartree-Fock level could also play an important role in the stability of the phases in Fig. 11.

In the projected model obtained by consistent derivation from the large-$U$ Hubbard Hamiltonian, we have been unable to find these states because of continued competition from superexchange terms, which are always significant. In this case the mutual frustration of the two competing interactions raises the possibility of further exotic spin configurations, such as the scalar-chirality phase,$^{25,26}$ or different dimerized structures breaking lattice translation symmetry.$^{25-28}$ However, with an arbitrary choice of large $K$ unrelated to the consistency considerations of Sec. IV, the same “three-up, one-down” phase emerges directly [Fig. 11(b)].

VI. SUMMARY AND CONCLUSIONS

In this contribution we have considered a microscopic description of circulating charge- and spin-current states in a planar model appropriate for cuprate systems, and the qualitative influence upon these phases of cyclic, four-spin interactions. The CF and SF phases were established on a small cluster by iterative solution for the electronic states within the HFA for the generalized Hubbard model. Although the real-space Hartree-Fock approach does not in general favor homogeneous and dynamically stabilized states, preferring localized and charge-inhomogeneous structures, meaningful qualitative comparisons remain possible.

The robust qualitative conclusions concerning flux phases are the following. CF and SF states are favored for small on-site repulsion $U$, and are stabilized primarily by next-neighbor superexchange ($J$) and Coulomb ($V$) contributions. They are most favorable close to half-filling, becoming unstable to non-ordered metallic phases at higher hole doping ($x > 0.15$ in HFA), a result which reflects qualitatively the onset of the Fermi-liquid phase.
beyond optimal doping in the cuprates. The bond current $J$ increases with interaction strength, tending in the limit $|J|/t, 4V/t \gg 1$ towards a $\pi$-flux phase in the CF state, and in the SF state to an imaginary bond order parameter preceding a ferromagnetic instability. Very few inhomogeneous current states are found in this type of analysis, and coexisting states are dominated by localized charge and magnetic configurations.

The inclusion of strong electronic correlations by projection of the hopping terms may yield solutions qualitatively different from those obtained for independent electrons in a weak-coupling treatment (unprojected hopping). Projected hopping is therefore essential in making contact with cuprate-relevant parameters. Inclusion of projection effects within the Gutzwiller approximation shows that the CF phase does become competitive for realistic cuprate interactions. The CF phase in the projected model has a clearly defined regime of stability at low and intermediate doping, in close correspondence to the underdoped and optimally doped regimes in cuprates. While projection produces very small kinetic terms near half-filling, it also pushes the general CF state towards a $\pi$-flux phase. Next-neighbor hopping contributions ($t'$) of the magnitude and sign relevant for cuprate systems appear to reinforce the projected CF phase. By contrast, the SF phase is excluded in a projected model, demonstrating that this type of flux phase is not compatible with strong electron correlations.

Introduction of a ring-exchange interaction $(K > 0)$ is detrimental to the stability of CF phases in both unprojected and projected models. By contrast, the SF phase shows an enhanced current and minimal energy penalty in the unprojected framework. Ring-exchange effects vary little with doping until the spin and bond order parameters are strongly reduced at high filling. The parameter values in cuprates are such that the $K$ term is largely irrelevant for qualitative phenomena at the Hartree-Fock level, and its effect remains weak even with the strong enhancement provided by the Gutzwiller approximation. However, we have shown that an exception to this statement arises for ordered magnetic states at very low filling, where the ring-exchange interaction might become qualitatively significant in a projected model.

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