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Circulating-current states and ring-exchange interactions in cuprates ☆

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Abstract

We consider circulating charge- and spin-current states in a generalised Hubbard model for the CuO$_2$ planes in cuprates. We investigate the parameter regimes for these phases in microscopic calculations on small clusters. We demonstrate that a positive ring-exchange interaction enhances (suppresses) spin- (charge-)flux phases.

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The possibility of phases supporting circulating currents has been recognised in two-dimensional (2D) models for the CuO$_2$ planes in cuprate materials since the advent of high-T_c superconductivity [1]. In addition to charge-flux (CF), or orbital antiferromagnetic, states, the same class of models also contains spin-flux (SF), or spin nematic, phases [2] (Fig. 1). Different forms of CF state have been proposed in the context of the "hidden order parameter" in the underdoped regime [3].

The possible significance of cyclic four-spin, or "ring-exchange", interactions in cuprates was also recognised at an early stage [4]. The magnitude of this contribution has been quantified by systematic expansions of Hubbard-type models, and is in good agreement with experiment [5].

We consider the extended Hubbard model

$$H = H_{\rm H} + H_{\rm J} + H_{\rm V} + H_{\rm K}, \tag{1}$$

where for nearest-neighbour bonds $\langle ij \rangle$

$$H_{\rm H} = -t \sum_{\langle ij\rangle\sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + {\rm H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{2}$$

$$H_{\rm J} + H_{\rm V} = J \sum_{\langle ij\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + V \sum_{\langle ij\rangle} n_i n_j, \tag{3}$$

$n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$ and $n_i = \sum_\sigma n_{i\sigma}$. The J and V terms in Eq. (3) correspond to superexchange and nearest-neighbour Coulomb interactions.

We work in real space (RS) on a finite, square cluster and adopt a Hartree–Fock (HF) decomposition of the interactions which admits finite average values of site charge $\langle n_i \rangle$, site magnetic moment $\langle \mathbf{S}_i \rangle$ and bond order

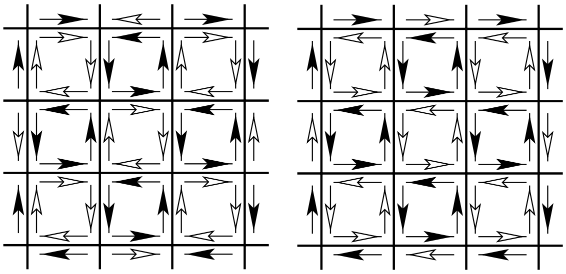

Fig. 1. Schematic representation of charge-flux (left) and spin-flux (right) phases. Solid (open) arrows represent currents of up (down) electrons.

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parameters $\langle c^{\dagger}_{i\sigma} c_{j\sigma} \rangle$ for bonds $\langle ij \rangle$. The RSHF approach has been used extensively for qualitative studies of stripe and other density-wave phases in cuprate systems [6], and requires careful selection of the initial state and the boundary conditions (BCs).

As expected from weak-coupling approaches [2], we establish the presence of CF states for $J > 0$ and SF states for $J < 0$, at large values ($\gtrsim 1$) of the interaction ratios $|J|/U$ and $4V/U$. The strong propensity within RSHF for charge localisation, driven by large U, and inhomogeneity and phase separation, driven by large $|J|$ and V, results in homogeneous CF or SF states only at a small number of doping values $x = 1 - n$ per site. These include 4, 12, 20, 22 and 30 holes in 12×12 systems with periodic BCs. At other values of x, inhomogeneous flux states coexist with magnetic moments and charge modulation. The ideal flux states exist only for small interactions at high x, and are robust for arbitrary interactions only at the lowest dopings. Thus CF and SF phases are destabilized as a function of x, and may be candidate ground states only close to $n = 1$.

The CF and SF states for 4 holes in a 12×12 system are characterised in Fig. 2(a), which shows the kinetic energy $T = \mathrm{Re}\langle c^{\dagger}_{i\sigma} c_{j\sigma} \rangle$ and current $I = \mathrm{Im}\langle c^{\dagger}_{i\sigma} c_{j\sigma} \rangle$ per bond for one spin direction σ. The interactions are fixed in the ratio $U = |J| = 4V$. Qualitatively, the current does not contribute to the kinetic energy, and the finite imaginary part is stabilised by Fock terms originating from decouplings of the J and V terms Eq. (3). Growth of the currents has little effect on T in Fig. 2(a), but while I_{CF} saturates with increasing interaction strength, I_{SF} continues to rise. Although the kinetic contribution remains nearly constant, the total energy increases monotonically in Fig. 2(b), reflecting the penalty for failure to adopt charge- or magnetically ordered states which destabilises the CF and SF phases.

The ring-exchange term takes the form

$$H_{\mathrm{K}} = \sum_{\square} K[(\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{S}_k \cdot \mathbf{S}_l) + (\mathbf{S}_i \cdot \mathbf{S}_l)(\mathbf{S}_j \cdot \mathbf{S}_k) - (\mathbf{S}_i \cdot \mathbf{S}_k)(\mathbf{S}_j \cdot \mathbf{S}_l)], \tag{4}$$

where $\square$ denotes the sum over the four spins $(ijkl)$ of each plaquette. This is decoupled into single-particle terms multiplied by all finite combinations of the remaining six operators, giving a structure similar to that of the J term. The effects of K may be assessed from the current and energy: it is clear from the currents [Fig. 2(c)] that $K > 0$ ($K < 0$) acts to suppress CF (SF) states. The energies E_{K} have the same sign as K (due to the quartic nature of the interaction), and are smaller for the SF state [Fig. 2(d)]. The conclusion that K favours a SF phase in a 2D lattice is consistent with recent observations from exact diagonalisation of small clusters. At large K one finds non-collinear magnetic phases with low bond kinetic energy but finite spin flux.

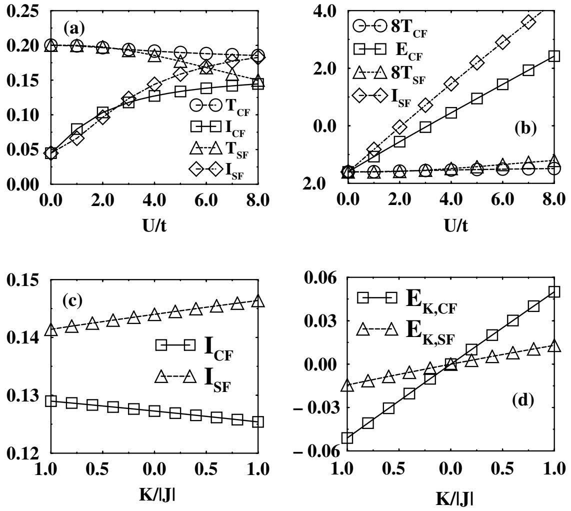

Fig. 2. Properties of CF and SF phases with $U = |J| = 4V$ and $K = 0$: (a) bond kinetic energy T and current I; (b) total energy E and kinetic energy $8T$; influence of K on CF and SF phases with $U = |J| = 4V = 4t$: (c) current I; (d) energy contribution E_{K}.

In summary, the RSHF technique for the extended Hubbard model shows that CF and SF phases exist for low U and only at low doping ($x \simeq 0$), where they are stabilised primarily by J and V interactions. A positive ring-exchange interaction K [5] enhances SF and suppresses CF states. However, parameter values for cuprates are such that K has only a very weak effect.

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