Charge density wave in the spin ladder of
$\text{Sr}_{14-x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41}$

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Abstract

We consider a multiband charge transfer model for a single spin ladder
describing the holes in $\text{Sr}_{14-x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41}$. Using Hartree-Fock approxi-
mation we show how the charge density wave, with its periodicity depen-
dent on doping as recently observed in the experiment, can be stabilized
by purely electronic many-body interactions.

A prerequisite for the understanding of high $T_c$ superconducting cuprates (HTSC)
is to describe the normal phase and its possible instabilities which may lead to
other ordered phases that compete with the superconducting one. As recently
investigated experimentally [1], such a competing phase in the hole doped weakly
coupled spin ladder system $\text{Sr}_{14-x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41}$ (SCCO) is the electronic charge
density wave (CDW). It is well known that CDW could in general be stabilized
due to either: (i) strong long-range or at least intersite Coulomb interaction,
or (ii) the Peierls instability, or (iii) charge stripe formation in the single-band
($t$-$J$) model [2]. However, the long-range Coulomb interaction is largely sup-
pressed in HTSC [3] and the Peierls origin of the CDW in SCCO is excluded [1].
Furthermore, the Zhang-Rice [4] derivation of the single band $t$-$J$ Hamiltonian
for HTSC is still controversial [5] and makes it questionable to explain charge
order (CO) in SCCO within the $t$-$J$ model. Hence it is puzzling to investigate
whether: (i) the $d$–$p$ multiband charge transfer model can explain the onset of
the CO in this compound by on-site Coulomb interactions alone, and (ii) the
calculated CDW periodicity agrees with the one observed experimentally and
hence could give strong theoretical support for the CDW in SCCO as induced
by electronic interactions.

The theoretical model for a decoupled single ladder [the weak coupling be-
tween the ladders can be neglected in leading order] includes seven orbitals
per Cu$O_5$ ladder unit cell (within Cu$O_3$ plane), and is similar to that de-
veloped earlier for Cu$O_2$ planes of HTSC [6]. The unit cell consists of: two
Cu(3d_{x^2-y^2} \equiv d) orbitals on two legs of the ladder, one bridge O(2p_\sigma \equiv b) orbital in the inner part of each ladder rung, two O(2p_\sigma \equiv p) orbitals on the ladder legs, and two other ones on outer parts of the rung (also labelled as p); cf. Fig. 1. The d and p orbitals belong to two sets for the right (R) and left (L) leg, respectively. We include large on-site Coulomb repulsion on copper (U) and oxygen (U_p), the charge transfer energy for the p orbitals, \( \Delta = \epsilon_p - \epsilon_d \), and for the b orbitals, \( \varepsilon = \varepsilon_b - \varepsilon_d \). For convenience we set \( \varepsilon_d = 0 \) and use the hole notation. Hence we consider the Hamiltonian,

\[
H = \left( - \sum_{m,j,\sigma} t_{mj} d_{m\sigma}^\dagger p_{j\sigma} - \sum_{m,\sigma} t_{mi} d_{m\sigma}^\dagger b_{i\sigma} + \text{h.c.} \right) + \Delta \sum_{j \in R,L} n_{pj} + \varepsilon \sum_i n_{bi} + U \sum_{m \in R,L} n_{m\uparrow} n_{m\downarrow} + U_p \left( \sum_i n_{bi\uparrow} n_{bi\downarrow} + \sum_{j \in R,L} n_{pj\uparrow} n_{pj\downarrow} \right),
\]

where \( t_{mj}, t_{mi} \) are the hopping elements between nearest neighbor pairs of \{p, d\} orbitals which include the respective phases, and \( n_{m} = \sum_{\sigma} n_{m\sigma}, n_{pj} = \sum_{\sigma} n_{pj\sigma}, n_{bi} = \sum_{\sigma} n_{bi\sigma} \) are particle number operators.

The model parameters (\( U = 9 \text{ eV}, U_p = 4.2 \text{ eV}, \Delta = 3.5 \text{ eV} \)) follow from ref. \[3\], whereas \( \varepsilon \) is somewhat smaller than \( \Delta \) \[7\]. Present value of \( t = 1 \text{ eV} \) is motivated by the experimental value of the superexchange constant \( J \) \[8\], though our results turn out to be valid for large range of the hopping parameter \( t \). SCCO is a self-doped compound with \( 1 < n < 1.33 \) (number of holes/Cu ion in the ladder) \[7\]. In the limit \( t \ll U \) one finds one hole in each \( d \) orbital and the antiferromagnetic (AF) order. Depending on the ratio \( \varepsilon/\Delta \) the doped holes go either to a linear combination of \( p/b \) orbitals, or to the \( b \) orbitals alone. Hence, in the regime of \( t \ll \{U, \Delta\} \) the kinetic exchange could favour the formation of: (i) Zhang and Rice (ZR) bound state \[4\], or (ii) a rung bound state with the hole being doped into \( b \) orbital and having an opposite spin to those of two neighboring holes in \( d \) orbitals. This means that for a commensurate hole doping \( \delta = n - 1 \) these states would naturally form a CDW of period \( l \) (Fig. 1), unless such bound states were not destabilized by increasing bandwidth.

In order to verify such a mechanism of CDW formation we studied the
energies of three different CO states (Fig. 1) determined self-consistently in the Hartree-Fock approximation, using $60 \times 7$ or $64 \times 7$ clusters. Stable CO insulating states have lower energies than a homogeneous AF state (not shown).

For $\varepsilon = \Delta$ one finds that: (i) both of the ZR states are stable whereas $|\text{RUNG}\rangle$ is unstable, (ii) $|\text{1ZR}\rangle$ state is slightly more favoured energetically than the $|2\text{ZR}\rangle$ state, (iii) the CDW periodicity in the ground state is $l = 1/(2\delta)$. With decreasing ratio $\varepsilon/\Delta$ the $|\text{1ZR}\rangle$ state evolves into a $|\text{RUNG}\rangle$ state which makes the CDW with one hole per rung even more robust. In this case one gains $(\Delta - \varepsilon)(\langle n_b \rangle - 0.5)$ on-site energy, where $\langle n_b \rangle \cong 1$ is the number of holes in $b$ orbital in the $|\text{RUNG}\rangle$ state.

We obtained that for $n = 1.2$ the CDW with period $l = 5$ is stable, and for $n = 1.33$ the CDW with less charge on every third rung $[l = (3)]$ is stable, which both agree with the experiment for $x = 0 \ [n = 1.2]$ and $x = 11 \ [n = 1.3]$ in SCCO [7]. Though, for $x = 4 \ [n = 1.25]$ the CO has not been observed. We suggest that in this case the CO could be destroyed due to weak interladder interaction, as the topology of the arrangement of the ladders in the plane does not allow for a homogeneous order with an even period.

In summary, we have shown how the CDW can be stabilized in SCCO in the charge transfer model for a Cu$_2$O$_5$ ladder due to on-site Coulomb interactions. In the relevant range of parameters the Fermi surface is unstable and the CO insulating state is formed by ZR or rung states. The obtained periodicities of the CO agree qualitatively with the experimental data.

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