Spin-Orbit Coupling and Spirals in Doped La$_2$CuO$_4$

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Spin-orbit coupling in doped La$_2$CuO$_4$ can result in (1) a novel electron-phonon coupling involving soft oxygen “tilting” phonons, and (2) stabilization of a commensurate antiferromagnetic state over a spiral state in the presence of a sufficiently large tilt distortion. This second effect may be responsible for the unusual electronic properties of La$_{1.88}$Ba$_{0.12}$CuO$_4$.

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Spin-orbit (SO) coupling can lead to anisotropic corrections to the superexchange interaction between localized spins in a Mott insulator. Such corrections, first studied phenomenologically by Dzyaloshinskii [1] and microscopically by Moriya [2], depend sensitively on lattice structure. For example, the tilt distortion in the low-temperature orthorhombic (LTO) phase of La$_2$CuO$_4$ gives rise to a Dzyaloshinskii-Moriya (DM) interaction which causes a small ferromagnetic moment to appear in each copper-oxide layer [3]. A potentially related fact is that La$_{2-x}$Ba$_x$CuO$_4$, at a doping of $x \sim 0.12$, undergoes a structural transition to a low-temperature tetragonal (LTT) phase [4] in which superconductivity is strongly suppressed if not completely destroyed [5,6], and recent muon spin-rotation measurements have shown an ordered moment forming on the copper sites [7]. Pickett, Cohen, and Krakauer [8] have argued that a change in electronic band structure in the LTT phase is responsible for these anomalies while Thio et al. [9] have suggested that the DM interaction may play some role. This has motivated us to consider the effects of SO coupling in a doped Mott insulator.

In this Letter we study a Hubbard model on a two-dimensional square lattice in which SO coupling appears as a small rotation of the electron spin as it hops between sites [10]. At half filling this small rotation results in a DM interaction which agrees with experiment [11]. Away from half filling we find that SO coupling gives rise to (i) a novel coupling between “tilting” phonons and electrons, and (ii) coherent nearest-neighbor hole hopping even in the presence of commensurate antiferromagnetic (AFM) order. This latter effect is similar to the coherent nearest-neighbor hopping which occurs in the various proposed spiral states [12-14] for which recent neutron scattering experiments on La$_{2-x}$Sr$_x$CuO$_4$ provide some experimental support [15]. We find that in the presence of a sufficiently large tilt distortion SO coupling can stabilize a commensurate AFM state over a spiral. Such a sudden change in magnetic structure may account for the unusual electronic properties of La$_{1.88}$Ba$_{0.12}$CuO$_4$.

A one-band Hubbard model may describe the essential low-energy electronic physics of a single copper-oxide layer [16]. The simplest generalization of such a model which includes SO coupling is

$$H = \sum_{\alpha,\beta} \{c_{\alpha}^{\dag}(-t\delta_{\alpha\beta} + i\lambda_{ij} \sigma_{\alpha\beta})c_{\beta}^{\dag} + \text{H.c.}\} + U \sum_{\alpha} n_{\alpha} n_{\alpha},$$

where $c_{\alpha}^{\dag}$ creates an electron with spin $\alpha$ at site $i$, $n_{\alpha} = c_{\alpha}^{\dag} c_{\alpha}$ is the corresponding number operator, and $\sigma_{\alpha\beta}$ is the vector of Pauli matrices. The lattice has $N$ sites and the number of electrons in the system is $N(1 - \delta)$. Hamiltonian (1) describes a correlated tight-binding band with hopping integral $t$ and on-site correlation $U$ in which SO coupling induces a spin precession of magnitude $|\lambda_{ij}|/t$ about $\lambda_{ij}$ when an electron hops from site $i$ to site $j$. The value of $\lambda_{ij}$ depends on the tilting pattern of the oxygen octahedra surrounding the copper ions. Figure 1 shows the pattern of oxygen displacements in the LTO and LTT phases in which the octahedra are rotated about the (110) and (100) axes, respectively. Symmetry alone dictates [17] that in the LTO phase

$$\lambda_{i,i+\hat{x}} = (-1)^{i_1 + i_3} \alpha_1 \lambda_2 0 / \sqrt{2},$$

$$\lambda_{i,i+\hat{y}} = (-1)^{i_3 + i_1} \alpha_3 \lambda_1 0 / \sqrt{2},$$

and in the LTT phase

$$+ + - -$$

| Cu | Cu | 0 | Cu | Cu | 0 |

$$- + - +$$

+ Cu - Cu + 0 Cu Cu 0

+ - LTO LTT

Fig. 1. Pattern of oxygen displacements in a single copper-oxide layer in (a) the LTO and (b) the LTT phases of doped La$_2$CuO$_4$. The symbols +, −, and 0 represent oxygen atoms which are, respectively, coming out of, going into, and lying in the copper-oxide plane.

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\[
\lambda_{l,i+\hat{x}} = (-1)^{l_x+i_y}\lambda_{l,i,0,0},
\]
\[
\lambda_{l,i+\hat{y}} = (-1)^{l_x+i_y}\lambda_{l,i,0,0},
\]
where \(l_x\) and \(l_y\) are the \(x\) and \(y\) coordinates of site \(i\) and \(\hat{x}\) and \(\hat{y}\) are unit vectors, all in units of the lattice spacing. Recent microscopic calculations [11] have shown that in both cases \(\lambda_1 = \gamma_1\theta\) and \(\lambda_2 = \gamma_2\theta\), where \(\gamma_2 > \gamma_1 > 0\), and \(\theta\) is the angle through which the octahedra are rotated. Although a nonzero \(\lambda_1 - \lambda_2\) is responsible for weak ferromagnetism in the LTO phase [18] in what follows we take \(\gamma_1 = \gamma_2 = \gamma\) so that the \(\lambda_{ij}\) are parallel to \((100)\) in the LTO phase and \((100)\) in the LTT phase [19]. As a rough estimate of the size of SO coupling in \(\La_2\CuO_4\) we take \(\gamma = (\Delta g/\eta)_{\nu}\) where \(g\) is the electron \(g\) factor and \(\Delta g\) is the shift in the \(g\) factor due to SO coupling. For \(t = 400\) meV and [3] \(\Delta g/\eta \sim 0.1\) one obtains \(\lambda = (40\) meV\()\theta\), so that in the LTO phase, where [3] \(\theta_{\LT}\sim 0.05\), we have \(\lambda_{\LT} \sim 2\) meV. Note that in the absence of SO coupling the interaction between octahedral sites and electrons is quadratic in \(\theta\) (Ref. [20]) so that the SO-induced \(\lambda_{ij}\), which is linear in \(\theta\), dominates for small \(\theta\).

Taking the \(x\) axis in spin-space parallel to the \(\lambda\) vectors in both the LTO and LTT phases allows (1) to be written

\[
H_{\text{eff}} = -i \sum_{\langle l,j \rangle_a} \left[ e^{i\phi_{l,j}} c_{l,a}^{\dagger} c_{j,a} + \text{H.c.} \right] + t' \sum_{\langle l,j,k \rangle} \left[ (c_{l,a}^{\dagger} \sigma_{a b} c_{j,b} S_j^a - i/2 c_{l,a} c_{k,b} H_i) e^{i(\theta_a + \theta_b) a} + (c_{l,a}^{\dagger} \sigma_{a b} c_{k,b} S_j^a - i/2 c_{l,a} c_{k,b} H_i) e^{-i(\theta_a - \theta_b) / 2} + \text{H.c.} \right] + J \sum_{\langle l,j \rangle_{\alpha \beta}} \left[ S_i^a S_j^a + \cos \phi_{l,j} (S_i^a S_j^a + S_i^b S_j^b) + \sin \phi_{l,j} (S_i^a S_j^b - S_i^b S_j^a) \right] - \frac{i}{2} n_i n_j,
\]

\[t' = i t / U, \quad J = 4 J t / U, \quad S_i = \frac{\lambda}{\text{H.c.}} (c_{l,a}^{\dagger} \sigma_{a b} c_{j,b} / 2, \quad S_i^\alpha = S_i^a - i S_i^b, \quad \sigma^\alpha = (\sigma^a + i \sigma^b) / 2, \quad \text{and} \quad \langle l,j,k \rangle \text{runs over all triplets of distinct sites where} \quad l,j,k \text{are nearest neighbors. \ Because of the alternating sign of} \quad \phi_{l,j} \text{the DM interaction is completely frustrated by the superexchange and no spin canting results} \quad \text{[17]. \ The anisotropic exchange then lines the spins up in the} \quad z \text{ direction so that they are parallel to} \quad (110) \text{in the LTO phase and} \quad (100) \text{in the LTT phase.}
\]

Away from half filling we apply a semiclassical approximation to (5) and consider the case where the spins lie in the \(x-y\) plane (i.e., perpendicular to the direction in which they point at half filling). First we define the operators \(a_i^\dagger = \exp(\pi n_i / 2) c_i^\dagger + \exp(-\pi n_i / 2) c_i\) and \(b_j^\dagger = \exp(\pi n_j / 2) c_j^\dagger - \exp(-\pi n_j / 2) c_j\) on the \(A\) and \(B\) sublattices, respectively. Then, if \(\{0\}\) denotes the state with no electrons, for \(n_\alpha = n_{\alpha,1} + n_{\alpha,2}\) the state \(|n_x, n_y\rangle = \sum_{\alpha,\beta} a_i^\dagger b_j^\dagger |0\rangle\) is a classical spiral [12–14] with pitch angles \(n_x\) and \(n_y\) in the \(x\) and \(y\) directions. When holes are added we make the mean-field replacements \(n_l \rightarrow (n_l) = 1 - \delta\) and \(S_i \rightarrow (S_i) = (-1)^{l_x+l_y} b_i / 2 \times (\cos n_i \sin n_i, 0)\) and diagonalize (5) within the Hilbert space spanned by states of the form \(\sum_{\alpha} a_{\alpha,1} b_{\alpha,2}^\dagger |\{n_x, n_y\}, \delta_{1,1}, \delta_{2,2}\rangle\), where \(\delta_{1,1} + \delta_{2,2} = \delta\). Doped holes then fill two bands (±) with dispersion \(E_{\pm} = \varepsilon_k \pm \varepsilon_k\), where

\[
\varepsilon_k = 2(1 - \delta) (t' \cos k_x + t' \cos k_y + 2 t' \cos k_x \cos k_y),
\]

with

\[
t' = t' \cos (\phi + n_x / 2) \cos (\phi - n_y / 2), \quad t' = t' \cos (\phi + n_y / 2) \cos (\phi - n_x / 2),
\]

\[
t' \geq t' \cos (\phi + n_x / 2) \cos (\phi - n_y / 2) + \cos (\phi - n_x / 2) \cos (\phi + n_y / 2),
\]

where

\[
\varepsilon_k = 2 t \sin^2 (\phi / 2) \cos (n_x / 2) \cos k_x - \cos (n_y / 2) \cos k_y \cos (\cos (n_x / 2) \cos k_x - \sin (n_y / 2) \sin k_y) \frac{1}{2}.
\]

If there is no spiral or SO coupling the two hole bands describe coherent next-nearest-neighbor hopping and are degener-
erate. Both SO coupling and spiraling allow for coherent nearest-neighbor hopping, thus mixing the bands, lifting their degeneracy, and allowing doped holes to gain energy by populating one band preferentially over the other. Denoting the occupied (hole) \( k \) states in the + and \(-\) bands for a given \( \delta \) as \{\( k^+ \)\} and \{\( k^- \)\} the total energy per site is

\[
E[\eta_x, \eta_y] = \sum_{k \in \{k^+\}} E_k^+ + \sum_{k \in \{k^-\}} E_k^- - \frac{J}{4} (1 - \delta)^2 \cos \phi (\cos \eta_x + \cos \eta_y) + 2 | \frac{e}{4}
\]

where the third term is the magnetic energy cost of canting the spins into a spiral. It is important to note that this semiclassical approximation does not adequately treat the subtle “polaron” effects which, among other things, renormalize the coherent bandwidth of a single hole from \( \sim \tilde{T} \) to \( \sim J \) [22]. In order to partially include these effects in our calculation we follow Shraiman and Sigija [12] and Kane et al. [14] and treat \( \phi \) as a phenomenological parameter on the order of \( J \). However, we expect that \( \lambda \sim \tilde{T} \phi \) will not be renormalized to \( \tilde{T} \phi \) when the spins are lying in the \( x-y \) plane because hole motion due to \( \lambda \) involves a spin flip and so it is not impeded by the AFM nature of the spin background. We therefore expect that \( \phi \) will be renormalized along with \( \tilde{T} \) in such a way that \( \tilde{T} \phi \) remains constant.

The coherent motion due to spiraling and SO coupling are physically very similar. In the spiral case total spin is conserved and a hole moving through the lattice sees a slowly precessing spin background because the spins have been canted away from perfect Néel order. In the SO case total spin is not conserved and a mobile hole again sees a precessing spin background, this time because the spin of the hole itself precesses as it moves through the lattice. However, there is an important difference between the spiral and SO band splittings \( \pm q \): The spiral splits strongest at \( (\pi/2, \pm \pi/2) \) while SO splits strongest at \( (\pi, 0) \). As a result the energy of the coherent motion due to SO coupling competes with that of the spiral as can be seen clearly in the limit of small \( \delta \), \( \eta \), and \( \phi \), where we find

\[
\Delta E[\eta_x, \eta_y] = E[\eta_x, \eta_y] - E[0,0]
\]

\[= \min [2\delta (|\phi| - |\eta_x| - |\eta_y|), 0]
\]

\[+ \frac{1}{2} J (\eta_x^2 + \eta_y^2) \).
\]

\( \Delta E[\eta_x, \eta_y] \) is minimized when \( \eta_x = \eta_y = 0 \) or \( \eta_x = \eta_y = \pm \phi \). The energy per site due to SO coupling \(-4(\delta \phi^2)/J \) is 4 times larger than the magnetic energy cost of moving the spins into the \( x-y \) plane \(-J\phi^2/4 \). Thus, as the size of the tilt distortion is increased there is an abrupt transition from a spiral with finite pitch to a commensurate AFM state. When this transition occurs the energy per site due to SO coupling is \(-4(\delta \phi^2)/J \). As the size of the tilt distortion is increased there is an abrupt transition from a spiral with finite pitch to a commensurate AFM state. When this transition occurs the energy per site due to SO coupling is \(-4(\delta \phi^2)/J \).

This effect may be responsible for the sudden change in electronic properties at the LTO \(-\) LTT structural transition in La_{1.88}Ba_{0.12}CuO_4. To investigate the plausibility of this we have minimized \( \delta \) for \( \delta = 0.125 \) using two (renormalized) values of \( \phi \), \( \phi_{\text{LTO}} = 0.04 \) and \( \phi_{\text{LTT}} = 0.16 \), taking \( J = 100 \) meV, \( \tilde{T} = 25 \) meV, and \( \tilde{T} = 50 \) meV so that \( \lambda_{\text{LTO}} \sim 2 \) meV and \( \lambda_{\text{LTT}} \sim 8 \) meV corresponding to distortion angles \( \beta_{\text{LTO}} \sim 0.05 \) and \( \beta_{\text{LTT}} \sim 0.2 \). We are therefore supposing that the distortion in the LTT phase is 4 times larger than in the LTO phase. Figure 2 shows the hole energy bands corresponding to the optimal spin configurations for these cases. In the LTO phase the spins form a spiral with pitch angles \( \eta_x \sim 0.16 \) and \( \eta_y \sim 0 \), the bands split at \( (\pi/2, \pm \pi/2) \), and the (hole) Fermi level lies in the gaps near these points so that the system gains sufficient kinetic energy to compensate the magnetic energy cost of spiraling. In the LTT phase the \( (\pi, 0) \) band splitting has increased because \( \phi \) has increased, holes have been shifted away from \( (\pi/2, \pm \pi/2) \), and the optimal spin back-
ground is commensurate with coherent nearest-neighbor hole motion occurring purely through SO coupling. Note that for this doping and these parameters the Fermi level lies in the SO-induced gap at \((\pi,0)\) in both the LTO and LTT phases so that the electronic energy of the system is lowered in the LTT phase by an amount of order \(\delta(\tilde{\alpha}_{\text{LTT}} - \lambda_{\text{LTO}})\sim 0.8 \text{ meV.} \) Although this energy gain is small it may help stabilize the LTT phase for \(\delta \sim 0.12.\) As more holes are added the Fermi level rises above the \((\pi,0)\) gap and the energy gain in the LTT phase becomes smaller. This is consistent with experiments showing the LTT instability is associated with the special doping value \(\delta \sim 0.12\) and not a special Ba concentration [23].

To conclude, we have investigated the role of SO coupling in doped \(\text{La}_2\text{CuO}_4\) finding that it (i) induces a “flux” coupling electrons to soft tilting phonons, and (ii) stabilizes a commensurate AFM state over a spiral in the presence of a sufficiently large tilt distortion. This commensuration effect may account for the unusual electronic properties of the LTT phase of \(\text{La}_{2-x}\text{Ba}_x\text{CuO}_4\) provided the distortion in that phase is significantly larger than in the LTO phase.

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[19] By performing the appropriate local rotations in spin space it is always possible to transform the \(\lambda_{ij}\) vectors into this convenient form. N. E. Bones, unpublished.