Spin-Orbit Coupling and Spirals in Doped La_2CuO_4

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(Received 25 October 1991)

Spin-orbit coupling in doped La_2CuO_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 $La_{1.88}Ba_{0.12}CuO_4$.

PACS numbers: 75.10.Jm, 74.65.+n, 74.70.Vy

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_2CuO_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 $La_{2-x}Ba_xCuO_4$, 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 $La_{2-x}Sr_xCuO_4$ 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

$$H=\sum_{\substack{\langle i,j\rangle\\ \alpha,\beta}}\{c_{i\alpha}^{\dagger}(-t\delta_{\alpha\beta}+i\boldsymbol{\lambda}_{ij}\cdot\boldsymbol{\sigma}_{\alpha\beta})c_{j\beta}+\text{H.c.}\}+U\sum_i n_{i\uparrow}n_{j\downarrow}\,, \quad (1)$$

where $c_{i\alpha}^{\dagger}$ creates an electron with spin α at site i, $n_{i\alpha}=c_{i\alpha}^{\dagger}c_{i\alpha}$ is the corresponding number operator, and $\boldsymbol{\sigma}_{\alpha\beta}$ 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 $\sim|\boldsymbol{\lambda}_{ij}|/t$ about $\boldsymbol{\lambda}_{ij}$ when an electron hops from site i to site j. The value of $\boldsymbol{\lambda}_{ij}$ 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 $(1\bar{1}0)$ and (100) axes, respectively. Symmetry alone dictates [17] that in the LTO phase

$$\begin{aligned}\boldsymbol{\lambda}_{i,i+\hat{x}}&=(-1)^{(i_x+i_y)}(\lambda_1,\lambda_2,0)/\sqrt{2}\,,\\ \boldsymbol{\lambda}_{i,i+\hat{y}}&=-(-1)^{(i_x+i_y)}(\lambda_2,\lambda_1,0)/\sqrt{2}\,,\end{aligned} \quad (2)$$

and in the LTT phase

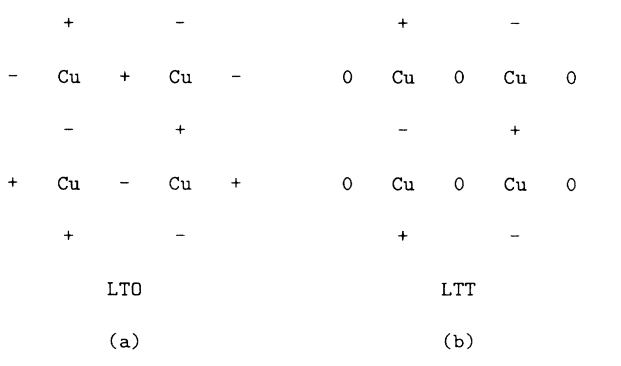

FIG. 1. Pattern of oxygen displacements in a single copper-oxide layer in (a) the LTO and (b) the LTT phases of doped La_2CuO_4. The symbols +, −, and 0 represent oxygen atoms which are, respectively, coming out of, going into, and lying in the copper-oxide plane.

$$\lambda_{i,i+\hat{x}}=(-1)^{(i_x+i_y)}(\lambda_1,0,0)\,,$$
$$\lambda_{i,i+\hat{y}}=-(-1)^{(i_x+i_y)}(\lambda_2,0,0)\,, \tag{3}$$

where i_x and i_y are the x and y coordinates of site i and $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ 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 θ 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 $\boldsymbol{\lambda}_{ij}$ are parallel to (110) in the LTO phase and (100) in the LTT phase [19]. As a rough estimate of the size of SO coupling in La_2CuO_4 we take $\gamma\sim(\Delta g/g)t$, where g is the electron g factor and Δg is the shift in the g factor due to SO coupling [2]. For [16] $t\sim400$ meV and [3] $\Delta g/g\sim0.1$ one obtains $\lambda\sim(40\text{ meV})\theta$, so that in the LTO phase, where [3] $\theta_{\rm LTO}\sim0.05$, we have $\lambda_{\rm LTO}\sim2$ meV. Note that in the absence of SO coupling the interaction between octahedral tilts and electrons is quadratic in θ (Ref. [20]) so that the SO-induced $\boldsymbol{\lambda}_{ij}$, which is linear in θ, dominates for small tilts.

Taking the z axis in spin-space parallel to the $\boldsymbol{\lambda}$ vectors in both the LTO and LTT phases allows (1) to be written [the spin index α in the exponent equals $+(-)\frac{1}{2}$ for spins parallel (antiparallel) to the z axis] as

$$H'=-\tilde{t}\sum_{\langle i,j\rangle\alpha}\{e^{i\phi_{ij}\alpha}c_{i\alpha}^{\dagger}c_{j\alpha}+\text{H.c.}\}+U\sum_i n_{i\uparrow}n_{i\downarrow}\,, \tag{4}$$

where $\tilde{t}=(t^2+\lambda^2)^{1/2}$, $\phi_{i,i+\hat{x}}=(-1)^{i_x+i_y}\phi$, and $\phi_{i,i+\hat{y}}=-(-1)^{i_x+i_y}\phi$, with $\phi=\arctan\lambda/t$. The Hamiltonian (4) describes electrons in the presence of a staggered fictitious "flux" in which up and down spin electrons have opposite fictitious "charge." This flux arises from the Berry's phase associated with the slow spin precession induced by the SO coupling and forms a staggered pattern because both the LTO and LTT distortions have wave vector (π,π). The magnitude of the flux is proportional to λ which is, in turn, proportional to θ, leading us to a natural speculation: The angle θ is associated with a soft phonon mode ($\omega\sim4$ meV) [20]. We anticipate that when this soft mode becomes thermally saturated it will give rise to a linear resistivity with the primary electron-phonon scattering mechanism being through SO-induced flux.

To study (4) when U/t is large we first perform a canonical transformation [21] to an effective strong-coupling Hamiltonian $H_{\rm eff}=P_dH'_{\rm eff}P_d$, where P_d is the Gutzwiller projection operator,

$$H'_{\rm eff}=-\tilde{t}\sum_{\langle i,j\rangle\alpha}\{e^{i\phi_{ij}\alpha}c_{i\alpha}^{\dagger}c_{j\alpha}+\text{H.c.}\}+t'\sum_{\langle i,j,k\rangle\alpha,\beta}\{(c_{i\alpha}^{\dagger}\sigma^z_{\alpha\beta}c_{k\beta}S_j^z-\tfrac{1}{2}c_{i\alpha}^{\dagger}c_{k\alpha}n_j)e^{i(\phi_{ij}+\phi_{jk})\alpha}+(c_{i\alpha}^{\dagger}\sigma^+_{\alpha\beta}c_{k\beta}S_j^-e^{i(\phi_{ij}-\phi_{jk})/2}+\text{H.c.})\}$$
$$+J\sum_{\langle i,j\rangle}\{S_i^zS_j^z+\cos\phi_{ij}(S_i^xS_j^x+S_i^yS_j^y)+\sin\phi_{ij}(S_i^xS_j^y-S_i^yS_j^x)-\tfrac{1}{4}n_in_j\}\,, \tag{5}$$

$t'=\tilde{t}^2/U$, $J=4\tilde{t}^2/U$, $\mathbf{S}_i=c_{i\alpha}^{\dagger}\boldsymbol{\sigma}_{\alpha\beta}c_{i\beta}/2$, $S_i^-=S_i^x-iS_i^y$, $\sigma^+=(\sigma^x+i\sigma^y)/2$, and $\langle i,j,k\rangle$ runs over all triplets of distinct sites where i,j and j,k are nearest neighbors. When $\delta=0$ only the last part of (5) plays any role. The terms proportional to $\sin\phi_{ij}$ and $\cos\phi_{ij}$ are, respectively, a DM interaction and an easy-axis anisotropy. Because of the alternating sign of ϕ_{ij} the DM interaction is completely frustrated by the superexchange and no spin canting results [17]. The anisotropic exchange then lines the spins up in the z direction so that they are parallel to (110) in the LTO phase and (100) 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 $a_i^{\dagger}=\exp(i\eta_i/2)c_{i\uparrow}^{\dagger}+\exp(-i\eta_i/2)c_{i\downarrow}^{\dagger}$ and $b_j^{\dagger}=i\exp(i\eta_j/2)c_{j\uparrow}^{\dagger}-i\exp(-i\eta_j/2)c_{j\downarrow}^{\dagger}$ on the A and B sublattices, respectively. Then, if $|0\rangle$ denotes the state with no electrons, for $\eta_i=\eta_xi_x+\eta_yi_y$ the state $|\eta_x,\eta_y\rangle=\prod_{i\in A}\prod_{j\in B}a_i^{\dagger}b_j^{\dagger}|0\rangle$ is a classical spiral [12–14] with pitch angles η_x and η_y in the x and y directions. When holes are added we make the mean-field replacements $n_i\to\langle n_i\rangle=1-\delta$ and $\mathbf{S}_i\to\langle\mathbf{S}_i\rangle=(-1)^{i_x+i_y}[(1-\delta)/2]\times(\cos\eta_i,\sin\eta_i,0)$ and diagonalize (5) within the Hilbert space spanned by states of the form $\prod_{n=1}^{\delta_1N}a_{i_n}\prod_{m=1}^{\delta_2N}b_{j_m}\times|\eta_x,\eta_y\rangle$, where $\delta_1+\delta_2=\delta$. Doped holes then fill two bands ($\pm$) with dispersion $E_{\mathbf{k}}^{\pm}=\epsilon_{\mathbf{k}}\pm q_{\mathbf{k}}$, where

$$\epsilon_{\mathbf{k}}=2(1-\delta)(t'_x\cos2k_x+t'_y\cos2k_y+2t'_{xy}\cos k_x\cos k_y)\,, \tag{6}$$

with

$$t'_x=t'\cos[(\phi+\eta_x)/2]\cos[(\phi-\eta_x)/2],\quad t'_y=t'\cos[(\phi+\eta_y)/2]\cos[(\phi-\eta_y)/2]\,,$$
$$t'_{xy}=t'\{\cos[(\phi+\eta_x)/2]\cos[(\phi-\eta_y)/2]+\cos[(\phi-\eta_x)/2]\cos[(\phi+\eta_y)/2]\}\,,$$

where

$$q_k=2\tilde{t}\{\sin^2(\phi/2)[\cos(\eta_x/2)\cos k_x-\cos(\eta_y/2)\cos k_y]^2+\cos^2(\phi/2)[\sin(\eta_x/2)\sin k_x+\sin(\eta_y/2)\sin k_y]^2\}^{1/2}\,. \tag{7}$$

If there is no spiral or SO coupling the two hole bands describe coherent next-nearest-neighbor hopping and are degen-

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) $\mathbf{k}$ states in the + and − bands for a given δ as $\{\mathbf{k}^+\}$ and $\{\mathbf{k}^-\}$ the total energy per site is

$$E[\eta_x,\eta_y]=\sum_{\mathbf{k}\in\{\mathbf{k}^+\}}E_k^+ + \sum_{\mathbf{k}\in\{\mathbf{k}^-\}}E_k^- - \frac{J}{4}(1-\delta)^2[\cos\phi(\cos\eta_x+\cos\eta_y)+2], \tag{8}$$

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 Siggia [12] and Kane *et al.* [14] and treat $\tilde{t}$ as a phenomenological parameter on the order of J. However, we expect that $\lambda\sim\tilde{t}\phi$ will *not* be renormalized to $J\phi$ when the spins are lying in the x-y plane because hole motion due to λ involves a spin flip and so it is not impeded by the AFM nature of the spin background. We therefore expect that ϕ 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 ($\pm q_{\mathbf{k}}$): 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 δ, η, and ϕ, where we find

$$\begin{aligned}\Delta E[\eta_x,\eta_y]&\equiv E[\eta_x,\eta_y]-E[0,0]\\&\simeq\min[\tilde{t}\delta(2|\phi|-|\eta_x|-|\eta_y|),0]\\&\quad+\tfrac{1}{8}J(\eta_x^2+\eta_y^2).\end{aligned}\tag{9}$$

$\Delta E[\eta_x,\eta_y]$ is minimized when $\eta_x=\eta_y=0$ or $\eta_x=\eta_y=4\delta\tilde{t}/J$ depending on whether ϕ is greater than or less than $\phi_c=2\delta\tilde{t}/J$. 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 $-4(\delta\tilde{t})^2/J$, 4 times larger than the magnetic energy cost of moving the spins into the x-y plane $[\sim J\phi_c^2/4=(\delta\tilde{t})^2/J]$. It follows that in the commensurate state the spins are driven into this plane so that the holes can gain the maximum energy possible from SO coupling.

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 (8) for $\delta=0.125$ using two (renormalized) values of ϕ, $\phi_{LTO}=0.04$ and $\phi_{LTT}=0.16$, taking $J=100$ meV, $t'=25$ meV, and $\tilde{t}=50$ meV so that $\lambda_{LTO}\sim 2$ meV and $\lambda_{LTT}\sim 8$ meV corresponding to distortion angles $\theta_{LTO}\sim 0.05$ and $\theta_{LTT}\sim 0.2$. 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 $\eta_y=0$, 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 ϕ has increased, holes have been shifted away from $(\pi/2,\pm\pi/2)$, and the optimal spin back-

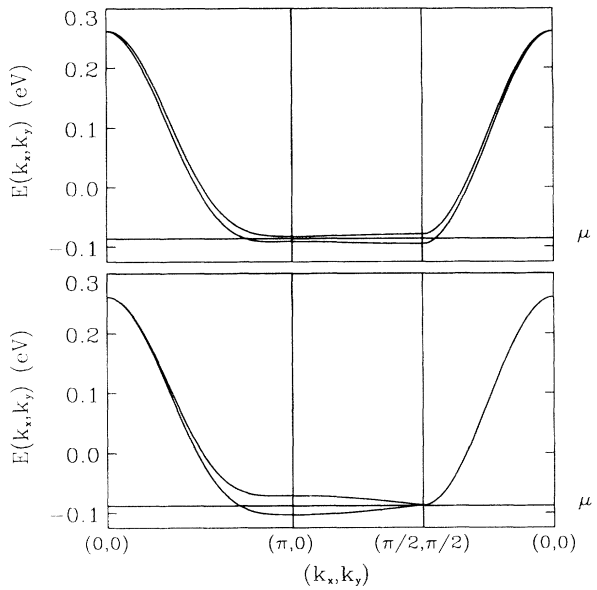

FIG. 2. Hole band structures showing band splitting from both spiraling and spin orbit (SO) for $J=100$ meV, $\tilde{t}=50$ meV, $t'=25$ meV, $\delta=0.125$, and $\phi=0.04$ (top), $\phi=0.16$ (bottom). In both cases the spiral pitch angles have been chosen to minimize Eq. (8). The horizontal lines labeled μ show the hole Fermi levels. For $\phi=0.04$ (LTO phase) the spins form a spiral with pitch angles $\eta_x\sim 0.16$ and $\eta_y=0$, splitting the bands at $(\pi/2,\pi/2)$ by ± 8 meV. The bands are also split due to SO at $(\pi,0)$ by ± 4 meV. For $\phi=0.16$ (LTT phase; assuming a factor of 4 increase in the distortion angle), the $(\pi,0)$ band splitting has increased to ± 16 meV, shifting holes away from $(\pi/2,\pi/2)$ so that there is no longer any energy gain from spiraling and $\eta_x=\eta_y=0$.

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 $\delta(\lambda_{LTT}-\lambda_{LTO})\sim 0.8$ 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 La_2CuO_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 $La_{2-x}Ba_xCuO_4$ provided the distortion in that phase is significantly larger than in the LTO phase.

One of us (N.E.B.) acknowledges useful discussions with J. Clayhold, M. Gingras, R. Hlubina, M. Ogata, and W. Putikka. We thank R. J. Gooding and J. W. Wilkins for helpful comments on the manuscript. This work was supported by the Swiss National Fund and NSF Grant No. DMR-89-13862.

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