

Electronic State of a CoO₂ Layer with Hexagonal Structure: A Kagomé Lattice Structure in a Triangular Lattice

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The electronic state in layered cobalt oxides with a hexagonal structure is examined. We find that the electronic structure reflects the nature of the Kagomé lattice hidden in the CoO₂ layer which consists of stacked triangular lattices of oxygen ions and of cobalt ions. A fundamental model for the electron system is proposed, and the mechanism of the unique transport and magnetic properties of the cobalt oxides are discussed in light of the model.

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Cobalt oxides with layered hexagonal structure have attracted much attention. The oxides Na_xCoO₂, (Bi,Pb)-Sr-Co-O, and Ca₃Co₄O₉ exhibit large thermopower and have potentials for thermoelectric materials [1–3]. In addition, the anomalous high-temperature Hall effect has been observed in Na_{0.68}CoO₂ [4]. It is known that Na_{0.75}CoO₂ shows a magnetic transition at 22 K [5], and (Bi,Pb)-Sr-Co-O is ferromagnetic below $T_C = 3.2$ K [6]. Recently, superconductivity [7] has been discovered in water-intercalated Na_{0.35}CoO₂ · 1.3H₂O. Since then, experimental and theoretical studies have been done extensively [4,8–20]. Several authors [17–20] have examined the electronic state based on a single band model in the triangular lattice of Co ions of the CoO₂ layer.

In this Letter we show that a Kagomé lattice structure is hidden in the CoO₂ layer, and the electronic state is based on the Kagomé lattice but not the single band model in the triangular lattice. We propose a fundamental model for the electron system and discuss the mechanism of the unique transport and magnetic properties in the cobalt oxides.

The crystal structure is presented in Fig. 1. The CoO₂ layer is formed by the edge-shared CoO₆ octahedra which are compressed along the *c* axis. The rhombohedral distortion of the CoO₆ octahedra are estimated by the deviation of the O-Co-O bond angle from 90°, 95°–99° [2,21–24]. The distortion leads to the crystal-field splitting in *t*_{2g} states of 3*d* electrons as shown in Fig. 1(c). The wave functions are expressed as

$$(|xy\rangle + |yz\rangle + |zx\rangle)/\sqrt{3} \quad (1)$$

for the *a*_{1g} state and

$$(|xy\rangle + e^{\pm i(2\pi/3)}|yz\rangle + e^{\pm i(4\pi/3)}|zx\rangle)/\sqrt{3} \quad (2)$$

for the doubly degenerate *e*'_g states where $|xy\rangle$, $|yz\rangle$, and $|zx\rangle$ denote the wave functions of the *t*_{2g} states. The *a*_{1g} state extends to the *c* axis, whereas the *e*'_g states spread over the plane perpendicular to the *c* axis. Since the apex oxygens approach the plane in the distorted CoO₆ octahedra, the *a*_{1g} state is stabilized [25] for an electron.

The band calculation [21] in Na_{0.5}CoO₂ has shown that the energy splitting between *a*_{1g} and *e*'_g states at the Γ point is ~ 1.6 eV which is the total bandwidth of the *t*_{2g} manifold and the *a*_{1g} state is higher than the *e*'_g states. This fact shows that the energy splitting does not originate in the crystal field due to the distortion but is determined by the kinetic energy of electrons.

Let us consider the hopping-matrix elements between neighboring 3*d* orbitals of cobalt ions neglecting the rhombohedral distortion. There are two mechanisms for the hopping of an electron: one is the hopping integral between adjacent 3*d* orbitals, and another is owing to the hopping between a 3*d* orbital of a cobalt ion and a 2*p* one of an oxygen ion. First, let us consider the latter mechanism, i.e., the hopping of a 3*d* electron through the 2*p* orbital on the neighboring oxygen. The CoO₂ layer in the hexagonal structure is expressed as a triangular lattice of cobalt ions sandwiched by those of oxygen ions; i.e., both the upper and lower layers of oxygens form triangular lattices. The lower layer is drawn by broken lines in Fig. 1(b). In the following, the *t*_{2g} orbitals on the *i*th cobalt ion are expressed as $|xy, i\rangle$, $|yz, i\rangle$, and $|zx, i\rangle$, respectively.

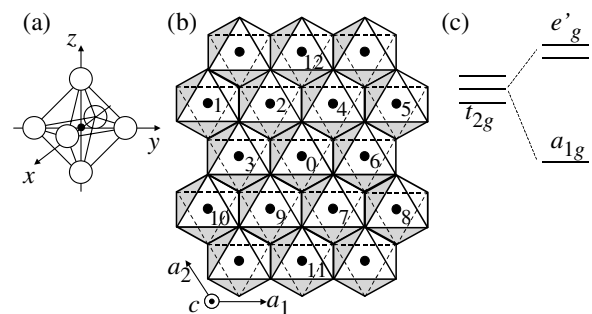


FIG. 1. (a) CoO₆ octahedron. Solid and open circles indicate cobalt and oxygen ions, respectively. (b) CoO₂ layer. *c* and *a*₁ axes are along the (1, 1, 1) and (−1, 1, 0) directions in the *xyz* coordinate system shown in (a). The numbers (0–12) on solid circles are the labels of Co sites. (c) The crystal-field splitting of the distorted CoO₆ octahedron. *e*'_g is used to distinguish from the *e*_g ($x^2 - y^2$ and $3z^2 - r^2$) states.

The CoO₆ octahedra share edges with each other, so that the Co-O-Co bond angle is $\pi/2$. The state $|zx, 0\rangle$ has a hopping matrix element with $|yz, 6\rangle$ through the $2p_z$ orbital of the oxygen ion which exists in the lower layer and shares CoO₆ octahedra involving cobalt ions 0 and 6, respectively. The hopping matrix element (t) is expressed as $t \sim (t_{pd})^2/\Delta (> 0)$, where Δ is the energy level of the $2p_z$ orbital measured from that of t_{2g} states and t_{pd} is the hopping integral between the $2p_z$ and $|zx, 0\rangle$ (or $|yz, 6\rangle$) orbitals. There also exists a hopping matrix element between $|yz, 0\rangle$ and $|zx, 6\rangle$ which is due to the $2p_z$ orbital of an oxygen ion on the upper layer. On the other hand, there is no hopping matrix element between $|xy, 0\rangle$ and $|xy, 6\rangle$ because of the symmetry. In the same way, we find the hopping matrix elements between the following pairs of orbitals: $(|xy, 0\rangle, |zx, 2\rangle)$, $(|zx, 0\rangle, |xy, 2\rangle)$, $(|xy, 0\rangle, |yz, 4\rangle)$, and $(|yz, 0\rangle, |xy, 4\rangle)$. In the Fourier-transformed representation, we have the tight binding Hamiltonian $H_t = \sum_{\vec{k}, \sigma, \gamma, \gamma'} \varepsilon_{\vec{k}, \gamma, \gamma'} c_{\vec{k}\sigma\gamma}^\dagger c_{\vec{k}\sigma\gamma'}$, with

$$\varepsilon_{\vec{k}} = 2t \begin{bmatrix} 0 & \cos(k_1 + k_2) & \cos k_2 \\ \cos(k_1 + k_2) & 0 & \cos k_1 \\ \cos k_2 & \cos k_1 & 0 \end{bmatrix}, \quad (3)$$

where k_1 and k_2 are the components of the wave vector \vec{k} of the triangular lattice spanned by \vec{a}_1 and \vec{a}_2 , respectively. The indices γ, γ' ($= xy, yz, zx$) and σ ($= \uparrow, \downarrow$) denote the t_{2g} orbitals and electron spin, respectively, and $c_{\vec{k}\sigma\gamma}^\dagger$ ($c_{\vec{k}\sigma\gamma}$) is the creation (annihilation) operator of an electron with \vec{k} , σ and γ (γ'). Equation (3) shows the well-known dispersion relation of the Kagomé lattice (see Fig. 2). This means that the Kagomé lattice structure stays in hiding in the triangular lattice of cobalt ions.

Let us discuss how to realize the Kagomé lattice in the motion of an electron given by Eq. (3). An electron in the state $|zx, 1\rangle$ can go to $|yz, 2\rangle$ and $|xy, 3\rangle$. An electron in $|yz, 2\rangle$ can go to $|xy, 12\rangle$ and $|xy, 3\rangle$ but cannot go to any orbitals on cobalt 0 due to the symmetry. In this way, an electron starting from $|zx, 1\rangle$ propagates through the t_{2g} orbitals on cobalt ions, 1–12, and thus the trace of the motion forms a Kagomé lattice [see Fig. 3(a)]. The triangle made of the states $|zx, 1\rangle$, $|yz, 2\rangle$, and $|xy, 3\rangle$ is an elementary unit of the Kagomé lattice. Therefore, the energy scheme of the triangle determines that at $(0, 0)$ in the k space. The eigenstates of the triangle are

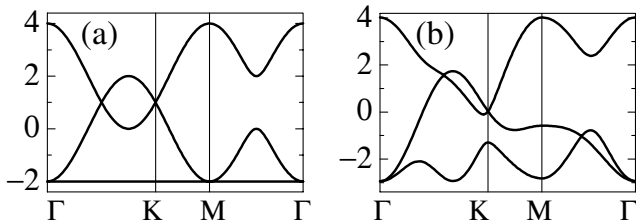


FIG. 2. (a) Dispersion relation of Eq. (3) for $t = 1$. (b) Dispersion relation of $E_{\vec{k}, \gamma, \gamma'}$ for $t = 1$, $t_{dd} = -0.63$, $t_1 = -0.08$, and $t_2/t_1 = -1.5$.

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$$(|xy, 3\rangle + |yz, 2\rangle + |zx, 1\rangle)/\sqrt{3} \quad (4)$$

with the eigenvalue $2t$ and

$$(|xy, 3\rangle + e^{\pm i(2\pi/3)}|yz, 2\rangle + e^{\pm i(4\pi/3)}|zx, 1\rangle)/\sqrt{3}, \quad (5)$$

with $-t$. The eigenstates correspond to the a_{1g} and e'_g symmetries, respectively. Note that they are completely different from the states Eqs. (1) and (2). The eigenstates in Eqs. (4) and (5) lie on the top and bottom of the band, respectively. This is a character of the Kagomé lattice structure.

When an electron propagates starting from $|yz, 1\rangle$, the trace can form another Kagomé lattice which is drawn by black triangles in Fig. 3(b). Following the procedure, we obtain four Kagomé lattices as shown in Fig. 3(b). Because the unit cell of the Kagomé lattice is 4 times as large as that of the triangular one, the four Kagomé lattices complete the Hilbert space.

In the CoO₂ layer where the CoO₆ octahedra share the edges as shown in Fig. 1, the hopping integral between adjacent 3d orbitals should also be taken into account to analyze the band structure. Between the cobalt ions 1 and 2, the leading term of the hopping matrix element (t_{dd}) occurs between $|xy, 1\rangle$ and $|xy, 2\rangle$. The sign of the hopping matrix element t_{dd} is negative due to the configuration of the orbitals on the hexagonal CoO₂ layer. Although there exist the other hopping matrix elements between the ions 1 and 2, e.g., between $|zx, 1\rangle$ and $|yz, 2\rangle$, their magnitude may be much smaller than the leading term. The hopping between xy orbitals forms a one-dimensional chain along the a_1 axis. In the same way, the hopping between yz (zx) orbitals forms another chain along the a_2 axis (the direction of $\vec{a}_1 + \vec{a}_2$). Consequently, the hopping matrix in the Fourier-transformed expression is diagonal; i.e., (xy, xy) , (yz, yz) , and (zx, zx) components are written as $2t_{dd} \cos(k_1)$, $2t_{dd} \cos(k_2)$, and $2t_{dd} \cos(k_1 + k_2)$, respectively. Note that the hopping matrix does not give the energy-level splitting at $(0, 0)$ in the k space.

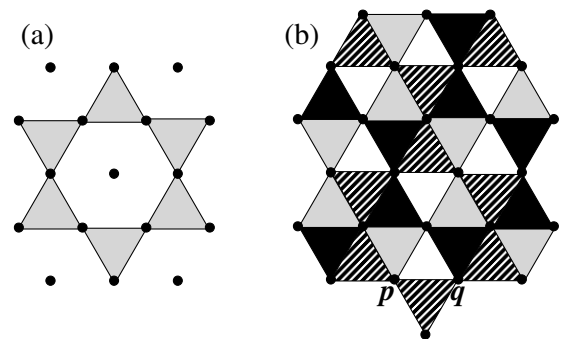


FIG. 3. Kagomé lattice in the triangular lattice of cobalt ions. (a) Solid circles indicate the cobalt ions in Fig. 1(b). Gray triangles form a Kagomé lattice which is made by a trace of the travel of an electron starting from $|zx, 1\rangle$ (see text). (b) Layout of the four (gray, black, hatched, and white) Kagomé lattices.

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For more detailed analysis, we introduce the effect of the hopping integral of $2p$ orbitals between neighboring oxygen ions. Let us consider the configuration of $2p$ orbitals on the oxygen ions labeled i–vi in Fig. 4 where the relation between xyz and a_1a_2c coordinate systems is the same as that in Fig. 1. The $2p_z$ orbitals on i, ii, and v are on an xy plane, but those on i and iii are not. Using the table by Slater and Koster [26], we find two kinds of hopping integrals as follows: $t_{pp,1} = V_{pp\pi}$ for

$$E_{\vec{k},\gamma,\gamma} = 2(t_{dd} + 2t_2) \cos k_a^{\gamma,\gamma} + 2(t_1 + 2t_2)[\cos k_b^{\gamma,\gamma} + \cos(k_a^{\gamma,\gamma} + k_b^{\gamma,\gamma})] - 2t_2[\cos(2k_a^{\gamma,\gamma} + k_b^{\gamma,\gamma}) + \cos(k_a^{\gamma,\gamma} - k_b^{\gamma,\gamma})],$$

$$E_{\vec{k},\gamma,\gamma'} = 2t \cos k_b^{\gamma,\gamma'} + 2t_1 \cos 2k_b^{\gamma,\gamma'} + 2t_2[\cos(k_a^{\gamma,\gamma'} + 2k_b^{\gamma,\gamma'}) + \cos(k_a^{\gamma,\gamma'} - k_b^{\gamma,\gamma'})],$$

where $k_a^{xy,xy} = k_a^{xy,zx} = k_1$, $k_b^{xy,xy} = k_b^{xy,zx} = k_2$, $k_a^{yz,yz} = k_a^{xy,yz} = k_2$, $k_b^{yz,yz} = k_b^{xy,yz} = -(k_1 + k_2)$, $k_a^{zx,zx} = k_a^{yz,zx} = -(k_1 + k_2)$, and $k_b^{zx,zx} = k_b^{yz,zx} = k_1$, respectively. The dispersion relation captures the band structure calculated by Singh [21]. Although more parameters may result in the more quantitative agreement with the band structure, it is not the purpose of this Letter.

The dispersion relation Fig. 2(b) clearly shows that the upper lying band takes over the nature of the Kagomé lattice structure hidden in the triangular lattice of cobalt ions (see Fig. 3) despite the presence of t_{dd} , t_1 , and t_2 . Therefore, it is of crucial importance to study the effect of the Kagomé lattice structure to clarify the electronic state in the CoO_2 layer.

So far, we have not discussed the effect of Coulomb interaction. In reality, the effective on-site Hubbard U of 5–8 eV is the largest scale of energy in the CoO_2 layer, and there exist Co^{3+} and Co^{4+} ions with the electronic configuration t_{2g}^6 and t_{2g}^5 , respectively. Let us discuss the effect of the strong Coulomb interaction in the Kagomé lattice structure shown in Fig. 3. The cobalt ions p and q are shared by white and hatched Kagomé lattices. The $3d$ orbitals $|yz, p\rangle$ and $|zx, q\rangle$ belong to the white Kagomé lattice, whereas $|zx, p\rangle$ and $|yz, q\rangle$ do in the hatched one. The on-site Coulomb interaction brings about the following interaction between p and q when an electron is in the

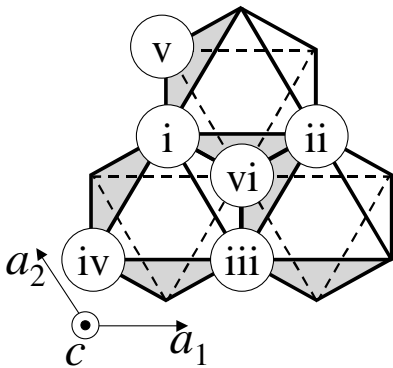


FIG. 4. Triangular lattices of oxygen ions in the CoO_2 layer. Cobalt ions are not drawn. i–iv (v and vi) are on the upper (lower) triangular lattice of oxygen ions.

the neighboring pair of oxygen ions, (i, ii) and (i, v), and $t_{pp,2} = (1/2)(V_{pp\sigma} + V_{pp\pi})$ for (i, iii), (i, iv), and (i, vi), where $V_{pp\sigma}/V_{pp\pi} = -4$, $t_{pp,2}/t_{pp,1} = -1.5$, and $t_{pp,1} < 0$. Following the procedure, all of the hopping integrals of $2p$ orbitals between neighboring oxygen ions are expressed as $t_{pp,1}$ and $t_{pp,2}$, which lead to the hopping matrix elements, t_1 and t_2 , of the $3d$ electron to the second nearest neighbors: $t_n \sim (t_{pd})^2 t_{pp,n}/(\Delta)^2$ where $n = 1$ or 2 . As a result, we obtain the hopping matrix $E_{\vec{k},\gamma,\gamma'}$ of the CoO_2 layer:

white Kagomé lattice and another is in the hatched one:

$$(\vec{T}_p \cdot \vec{T}_q - \frac{1}{4})[J(\vec{S}_p \cdot \vec{S}_q + \frac{3}{4}) + J'(\vec{S}_p \cdot \vec{S}_q - \frac{1}{4})],$$

where \vec{S}_p (\vec{S}_q) is the electron spin on p (q). The orbital state on p (q) is described by the pseudospin operator \vec{T}_p (\vec{T}_q) with $1/2$ in magnitude; i.e., $|yz, p\rangle$ ($|zx, p\rangle$) is the eigenstate of T_p^z with the eigenvalue $1/2$ ($-1/2$) and $|zx, q\rangle$ ($|yz, q\rangle$) is the eigenstate of T_q^z with the eigenvalue $1/2$ ($-1/2$). The interactions J and J' are expressed as $J = 4t^2/(U' - K)$ and $J' = 4t^2/(U' + K)$ with the Coulomb interaction U' of the interorbitals and Hund's rule coupling K . Because of the Hund's rule coupling, $J > J'$; i.e., there exists a ferromagnetic spin coupling with a singlet state of orbitals on the edge shared by the Kagomé lattices.

We propose a fundamental model to study the electronic structure of the CoO_2 layer under the local constraint, $\sum_{\sigma\gamma} c_{i\sigma\gamma}^\dagger c_{i\sigma\gamma} \geq 5$. The Hamiltonian $H = H_i + H_J$ with

$$H_J = \sum_{nm} (H_{2n\vec{u}+m\vec{v}}^{(1)} + H_{m\vec{u}+2n\vec{v}}^{(2)} + H_{2n(\vec{u}+\vec{v})+m\vec{v}}^{(3)}),$$

where n and m are integer numbers and

$$H_i^{(I)} = J \sum_{\vec{\delta}(I)} \left(\vec{T}_i^{(I)} \cdot \vec{T}_{i+\vec{\delta}(I)}^{(I)} - \frac{1}{4} n_i^{(I)} n_{i+\vec{\delta}(I)}^{(I)} \right) \times \left(\vec{S}_i \cdot \vec{S}_{i+\vec{\delta}(I)} + \frac{3}{4} n_i^{(I)} n_{i+\vec{\delta}(I)}^{(I)} \right),$$

where I is an index and $\vec{\delta}(1) = \pm \vec{a}_1$, $\vec{\delta}(2) = \pm \vec{a}_2$, and $\vec{\delta}(3) = \pm(\vec{a}_1 + \vec{a}_2)$ in the summation. The orbitals corresponding to the eigenstates of $T_i^{(I),z}$ are summarized in Table I, and $n_i^{(I)} = n_{i+}^{(I)} + n_{i-}^{(I)}$ where $n_{i\pm}^{(I)}$ is the electron number in the eigenstates of $T_i^{(I),z}$.

This model involves the ingredients for the unique transport and magnetic properties of the CoO_2 layer: A spin triplet with an orbital singlet is stabilized on a nearest-neighbor cobalt bond. The pairing mechanism acts in a different way from the so-called resonating-valence-bond picture discussed by several authors [17–20], where the key is the singlet state of orbitals.

TABLE I. Relation between t_{2g} (xy , yz , and zx) orbitals and eigenstates of $T_i^{(l),z}$ with $i = n\vec{a}_1 + m\vec{a}_2$. The letters with (without) the brackets denote the orbitals corresponding to the eigenstates in the case that $n + m$ is odd (even).

Eigenvalue	1/2	-1/2
$I = 1$	yz (zx)	zx (xy)
$I = 2$	zx (xy)	xy (zx)
$I = 3$	xy (yz)	yz (xy)

Khaliullin and Maekawa [27] discussed a liquid state of t_{2g} orbitals in a perovskite titanate. In the CoO_2 layer, the resonance and dynamics of the singlet states are developed in the Kagomé lattice but not in the triangular lattice. Note that the orbitals are characterized by four flavors, i.e., the four Kagomé lattices as shown in Fig. 3(b), rather than three t_{2g} states. This system has ferromagnetic interaction H_J . Thus, the carrier doping may cause a spin-triplet superconductivity [11–14]. This is based on the Kagomé lattice structure and is different from that on a single band model in a triangular lattice.

The Kagomé lattice involves a triangle as a basic unit. On the triangle, the mechanism by Kumar and Shastry [17,28] for the anomalous Hall effect is available and explains the experiments by Wang *et al.* [4].

The triangle gives the a_{1g} state Eq. (4) as the upper lying band in the reciprocal space. In the real space, however, a cobalt ion in the triangle is shared by three Kagomé lattices (see Fig. 3), so that the three t_{2g} orbitals are identical. The orbital degree of freedom causes the large thermopower [29,30] at high temperatures.

The Kagomé lattice structure clearly explains the non-symmetric nature of the band structure of the CoO_2 layer. When the effect of the Kagomé lattice becomes dominant, the bottom band, i.e., the flat band as shown in Fig. 2(a), will play a crucial role on the electronic state. Mielke [31] has shown that the flat band with the Coulomb interaction has the ferromagnetic ground state at around half filling. A prospective system for the ferromagnet will be d^1 transition metal oxides, i.e., the layered titanates with isostructure of the cobalt oxides. Although there exist many effects which disturb the flat band structure in reality, exploring the ferromagnet based on the mechanism will be a challenging problem.

In summary, we have shown that the Kagomé lattice structure is hidden in the CoO_2 layer. The electronic structure strongly reflects the nature of the Kagomé lattice but not the single band model with a triangular lattice. We have proposed a fundamental model for the electron system and discussed the mechanism of the unique transport and magnetic properties of the cobalt oxides.

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