

Topological band structure due to modified Kramers degeneracy for electrons in a helical magnetic field

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Two theorems on electron states in helimagnets are proved. They reveal a Kramers-like degeneracy in a helical magnetic field. Since a commensurate helical magnetic system is transitionally invariant with two multiple periods (ordinary translations and generalized ones with rotations), the band structure turns out to be topologically nontrivial. Together with the degeneracy, this gives an unusual spin structure of electron bands. A two-dimensional model of nearly free electrons is proposed to describe conductive hexagonal palladium layers under an effective field of magnetically ordered CrO₂ spacers in PdCrO₂. The spin texture of the Fermi surface leads to abnormal conductivity.

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Metallic delafossites PtCoO₂, PdCoO₂, and PdCrO₂ are layered compounds with anomalous transport properties [1–4]. Their conductivity at room temperature approaches that of the best elementary conductors such as silver, copper, and aluminum [1]. CoO₂ and CrO₂ are proved to be dielectric interlayers [5], and the conductivity in these substances is determined entirely by hexagonal palladium or platinum layers. This leads to extremely large values of the electron mean free path, up to 20 μm at low temperatures [4]. When electron momentum-relaxing scattering by impurities or phonons is much weaker as compared to momentum-conserving scattering, a hydrodynamic regime of electron transport appears [6], as it was observed in PdCoO₂ [7]. The unusual behavior of the delafossites suggests a novel mechanism of electron transport [8].

A long-range magnetic order appears in PdCrO₂ below $T_c = 37.5$ K [9–11]. Chromium ions form a 120° magnetic structure within a single layer. A complex interlayer arrangement leads to the magnetic system consisting of 18 sublattices [10]. The appearance of the magnetic order is accompanied by a resistivity drop [12]. Thus, a main hypothesis, which is going to be proved in the present Letter, is that the helical magnetic order on certain conditions induces a high-conductivity state. It also should be mentioned that an unconventional anomalous Hall effect [13] and nonreciprocal electronic transport [2] are observed in PdCrO₂ in the magnetically ordered state. Above T_c a short-range magnetic order in chromium hexagonal layers persists up to about 500 K [11,12], and this is another surprising fact in view of the extremely high conductivity.

The Fermi surface in the metallic delafossites was thoroughly investigated [1,4]. In the paramagnetic state, it is quasi-two-dimensional with a single α orbit. The transition to the ordered state in PdCrO₂ leads to a reconstruction of the Fermi surface within the magnetic Brillouin zone and the appearance of additional γ orbits corresponding to pockets in the vicinity of the K points [11,14].

The motion of a spin-1/2 particle in a helical magnetic field has been studied for a long time [15–20]. In particular, an exact solution is known [16] and there are various approximate approaches [17,21]. The electron transport in noncollinear magnetic structures is demonstrated to be nonreciprocal due to the breaking of spatial inversion symmetry [2,19]. A spin space group (SSG) theory is a useful instrument for the investigation of helical magnetic systems [22–24]. A SSG operator $\{\alpha|\beta|\mathbf{t}\}$ comprises the spin rotation α_s and space transformation $\{\beta|\mathbf{t}\}$ combining the rotation β and translation \mathbf{t} . In the framework of the theory, generalized translations are introduced ($\{\alpha|0|\mathbf{t}\}$), and a generalized Bloch theorem was proved [22,23].

The topological aspects of the band structure of crystalline solids were intensively studied during the last decades [25]. The main efforts of theoreticians and experimenters were concentrated on investigations of topological insulators and their edge states [26,27]. Another problem that was thoroughly studied was a Kramers-type degeneracy in various magnetic and topological systems [28]. Recently, magnetic topological insulators and semimetals including helimagnets turned out to be the focus of attention [29,30]. In the present Letter, another approach to the topology of metallic helimagnets is proposed.

Let us consider a particle of spin-1/2 in a nonuniform magnetic field, which is invariant under translation with period \mathbf{T} , i.e., $\mathbf{h}(\mathbf{r} + \mathbf{T}) = \mathbf{h}(\mathbf{r})$. The Hamiltonian of the system has the form

$$\hat{H} = \hat{H}_0 + \mathbf{h}(\mathbf{r})\hat{\sigma}, \quad (1)$$

where $\hat{\sigma}$ are the Pauli matrices. One can prove two theorems on the eigenvalues of the Hamiltonian.

Theorem 1. If \hat{H}_0 is invariant under the operation $\hat{\mathbf{T}}_{1/2}\hat{\theta}$, where $\hat{\mathbf{T}}_{1/2}$ is the space translation along vector $\mathbf{T}/2$, $\hat{\theta}$ is the time-reversal operator, and $\mathbf{h}(\mathbf{r} + \mathbf{T}/2) = -\mathbf{h}(\mathbf{r})$, then the eigenvalues $\varepsilon_{\mathbf{k}}$ of \hat{H} are at least twofold degenerate for all the wave vectors \mathbf{k} except those which satisfy $\exp(i\mathbf{k}\mathbf{T}) = -1$,

and the following condition is fulfilled for all the eigenvalues,

$$\varepsilon_{\mathbf{k},(\sigma)} = \varepsilon_{-\mathbf{k},-(\sigma)}, \quad (2)$$

where $(\sigma) \equiv \langle \psi_{\mathbf{k}} | \hat{\sigma} | \psi_{\mathbf{k}} \rangle$ and $|\psi_{\mathbf{k}}\rangle$ is the eigenstate of \hat{H} .

Proof. In the presence of a magnetic field a symmetry operation containing $\hat{\theta}$ should be a product of an operation, which changes the sign of the magnetic field, and $\hat{\theta}$ [31]. Therefore, $\hat{\mathbf{T}}_{1/2}\hat{\theta}$ is a symmetry operation for \hat{H} . Let us consider two eigenstates: $|\psi_{\mathbf{k}}\rangle$ and $\hat{\mathbf{T}}_{1/2}\hat{\theta}|\psi_{\mathbf{k}}\rangle$. According to the rules for antiunitary operators [32] we obtain

$$\begin{aligned} \langle \psi_{\mathbf{k}} | (\hat{\mathbf{T}}_{1/2}\hat{\theta} | \psi_{\mathbf{k}}) \rangle &= \overline{\langle \psi_{\mathbf{k}} | \hat{\theta}^\dagger (\hat{\mathbf{T}}_{1/2}\hat{\theta}^2 | \psi_{\mathbf{k}}) \rangle} \\ &= -\langle \psi_{\mathbf{k}} | \hat{\mathbf{T}}^\dagger (\hat{\mathbf{T}}_{1/2}\hat{\theta} | \psi_{\mathbf{k}}) \rangle. \end{aligned} \quad (3)$$

By means of Bloch's theorem $\hat{\mathbf{T}}|\psi_{\mathbf{k}}\rangle = \exp(i\mathbf{k}\mathbf{T})|\psi_{\mathbf{k}}\rangle$ it is reduced to

$$\langle \psi_{\mathbf{k}} | (\hat{\mathbf{T}}_{1/2}\hat{\theta} | \psi_{\mathbf{k}}) \rangle = -\exp(i\mathbf{k}\mathbf{T})\langle \psi_{\mathbf{k}} | (\hat{\mathbf{T}}_{1/2}\hat{\theta} | \psi_{\mathbf{k}}) \rangle. \quad (4)$$

From here one can see that $|\psi_{\mathbf{k}}\rangle$ and $\hat{\mathbf{T}}_{1/2}\hat{\theta}|\psi_{\mathbf{k}}\rangle$ are orthogonal and make up a pair of degenerate states for all \mathbf{k} except those which satisfy $\exp(i\mathbf{k}\mathbf{T}) = -1$. In the last case, the state can be either degenerate or nondegenerate. Since operators $\hat{\mathbf{k}}$ and $\hat{\sigma}$ commute with $\hat{\mathbf{T}}_{1/2}$ and change sign under the time reversal, we obtain Eq. (2). ■

The first term of Eq. (1) can contain a scalar potential and kinetic energy contribution $\hat{\mathbf{p}}^2/(2m)$ where $\hat{\mathbf{p}}$ and m are the momentum operator and particle mass. If the vector potential corresponding to $\mathbf{h}(\mathbf{r})$ has the same translational symmetry under a proper calibration [33], i.e., $\mathbf{A}(\mathbf{r} + \mathbf{T}/2) = -\mathbf{A}(\mathbf{r})$, the kinetic term can be extracted from \hat{H}_0 and the Hamiltonian

$$\hat{H} = \hat{H}_0 + [\hat{\mathbf{p}} + q_0\mathbf{A}(\mathbf{r})\hat{\mathbf{T}}]^2/(2m) + \mathbf{h}(\mathbf{r})\hat{\sigma} \quad (5)$$

also meets the theorem. Here, q_0 is the charge of the particle and $\hat{\mathbf{T}}$ is the unit matrix.

Helical systems with the SSG symmetry operator $\{\alpha|0|\mathbf{t}\}$, where $\alpha = 2\pi/n$ and n is an even natural number, satisfy the hypothesis of the theorem if $\mathbf{h}(\mathbf{r})$ is perpendicular to the axis of spin rotation. This can be illustrated by an example of a tight-binding model for a four-sublattice helical structure [see Supplemental Material (SM) [34]]. On the other hand, the theorem cannot be applied if n is the odd number, in particular, in the important case of 120° magnetic ordering ($n = 3$).

Let us introduce an operator $\hat{\mathbf{r}}_\alpha$ of spin rotation by angle α about the z axis. In the theorem and models discussed below, there is no spin-orbit coupling. Therefore, the spin rotation axis can be chosen to be arbitrary, i.e., it is independent of the spatial z' axis.

Theorem 2. If \hat{H}_0 in Eq. (1) is invariant under translation $\hat{\mathbf{t}}$, time reversion $\hat{\theta}$, and arbitrary rotations of the spin system about the z axis, and if $\mathbf{h}(\mathbf{r})\hat{\sigma}$ is invariant under $\hat{\mathbf{r}}_\alpha\hat{\mathbf{t}}$, where $\alpha = 2\pi/n$, n is an odd number ($n > 1$), and $\mathbf{h}(\mathbf{r})$ is perpendicular to the spin rotation axis, then the eigenvalues of \hat{H} are at least twofold degenerate for all the wave vectors \mathbf{k} except those which satisfy $\exp(2i\mathbf{k}\mathbf{T}) = 1$, where $\mathbf{T} = n\mathbf{t}$, and all the eigenvalues satisfy Eq. (2) with $\langle \hat{\sigma}_{x(y)} \rangle_{\mathbf{k}} = 0$.

Proof. Let us introduce the operators

$$\hat{\mathbf{Y}} = \hat{\mathbf{t}}\hat{\mathbf{r}}_\alpha \text{ and } \hat{\mathbf{X}} = \hat{\mathbf{t}}\hat{\mathbf{r}}_{\alpha-\pi}\hat{\theta}. \quad (6)$$

$\hat{\mathbf{Y}}$ is a symmetry operator under the hypothesis of the theorem and a generator of an Abelian group [23]. Its irreducible

representations coincide with those of the space translation group $\exp(i\mathbf{k}\mathbf{t})$, where \mathbf{k} is the wave vector in the extended Brillouin zone [23]. The magnetic field is perpendicular to the spin rotation axis, then $\hat{\mathbf{r}}_{-\pi}\mathbf{h}(\mathbf{r}) = -\mathbf{h}(\mathbf{r})$ and $\hat{\mathbf{X}}$ is also a symmetry operator. We can consider the following quantity:

$$\langle \psi_{\mathbf{k}} | (\hat{\mathbf{X}}^n | \psi_{\mathbf{k}}) \rangle = \langle \psi_{\mathbf{k}} | (\hat{\mathbf{X}}^{-n} | \psi_{\mathbf{k}}) \rangle. \quad (7)$$

Direct translations give

$$\begin{aligned} \langle \psi_{\mathbf{k}} | (\hat{\mathbf{t}}^{-n}\hat{\mathbf{r}}_{\alpha-\pi}^{-n}\hat{\theta}^{-n} | \psi_{\mathbf{k}}) \rangle &= \langle \psi_{\mathbf{k}} | \hat{\mathbf{t}}^{-2n}(\hat{\mathbf{t}}^n\hat{\mathbf{r}}_{\alpha-\pi}^{-n}\hat{\theta}^{-n} | \psi_{\mathbf{k}}) \rangle \\ &= -\langle \psi_{\mathbf{k}} | \hat{\mathbf{t}}^{-2n}\hat{\mathbf{r}}_{\alpha-\pi}^{-2n}(\hat{\mathbf{t}}^n\hat{\mathbf{r}}_{\alpha-\pi}^n\hat{\theta}^n | \psi_{\mathbf{k}}) \rangle. \end{aligned} \quad (8)$$

Using $\hat{\mathbf{r}}_{\alpha-\pi}^{-2n} = -\hat{\mathbf{T}}$ and Bloch's theorem $\hat{\mathbf{T}}^2|\psi_{\mathbf{k}}\rangle = \exp(2i\mathbf{k}\mathbf{T})|\psi_{\mathbf{k}}\rangle$, we obtain

$$\langle \psi_{\mathbf{k}} | (\hat{\mathbf{X}}^n | \psi_{\mathbf{k}}) \rangle = \exp(-2i\mathbf{k}\mathbf{T})\langle \psi_{\mathbf{k}} | (\hat{\mathbf{X}}^n | \psi_{\mathbf{k}}) \rangle. \quad (9)$$

That is, $|\psi_{\mathbf{k}}\rangle$ and $\hat{\mathbf{X}}^n|\psi_{\mathbf{k}}\rangle$ are orthogonal and the eigenstates are twofold degenerate for all the wave vectors except those which satisfy $\exp(2i\mathbf{k}\mathbf{T}) = 1$. The operators $\hat{\mathbf{k}}$ and $\hat{\sigma}_z$ commute with $\hat{\mathbf{t}}$ and $\hat{\mathbf{r}}$, as well as change sign under the time reversal. Therefore, we obtain $\varepsilon_{\mathbf{k},(\sigma_z)} = \varepsilon_{-\mathbf{k},-(\sigma_z)}$. The relations for the transverse spin components are proved in SM [34]. ■

If the vector potential has the same translational symmetry as $\mathbf{h}(\mathbf{r})$, i.e., $\hat{\mathbf{r}}_\alpha\hat{\mathbf{t}}\mathbf{A}(\mathbf{r}) = \mathbf{A}(\mathbf{r})$ [33], the Hamiltonian of the form (5) also satisfies Theorem 2.

Let us consider a tight-binding model of an atomic chain under an effective magnetic field corresponding to the 120° order as an example of a one-dimensional (1D) helical system satisfying Theorem 2,

$$\begin{aligned} \hat{H}_{3sl} = & -\sum_{i,\sigma} (\hat{a}_{i,1,\sigma}^\dagger \hat{a}_{i,2,\sigma} + \hat{a}_{i,2,\sigma}^\dagger \hat{a}_{i,3,\sigma} \\ & + \hat{a}_{i,3,\sigma}^\dagger \hat{a}_{i+1,1,\sigma} + \text{H.c.}) - \sum_{i,j,\sigma,\sigma'} (\hat{a}_{i,j,\sigma}^\dagger \hat{\mathbf{h}}_j \hat{a}_{i,j,\sigma'}), \end{aligned} \quad (10)$$

where $\hat{a}_{i,j,\sigma}^\dagger$ ($\hat{a}_{i,j,\sigma}$) is the electron creation (annihilation) operator in the j th sublattice ($j = 1, 2, 3$) and i th cell with the spin projection on the z axis $\sigma = \pm 1/2$. The on-site magnetic field for the sublattices is defined as follows: $\hat{\mathbf{h}}_1 = h_0\hat{\sigma}_x$, $\hat{\mathbf{h}}_2 = h_0(-\hat{\sigma}_x + \sqrt{3}\hat{\sigma}_y)/2$, $\hat{\mathbf{h}}_3 = h_0(-\hat{\sigma}_x - \sqrt{3}\hat{\sigma}_y)/2$.

This model is exactly solvable and the electron dispersion is shown in Fig. 1. The magnetic Brillouin zone lies between $-\pi$ and π . According to Theorem 2, the obtained eigenvalues obey Eq. (2). Special points, where the degeneracy is undefined ($k = 0$ and $k = \pm\pi$), are shown by yellow and green circles.

As was mentioned above, the helical system is subject to both the generalized Bloch theorem due to invariance under the generalized translation $\hat{\mathbf{r}}_\alpha\hat{\mathbf{t}}$ [22,23] and the ordinary Bloch theorem [35] (translational invariance under $\hat{\mathbf{T}} = \hat{\mathbf{t}}^n$). Therefore, the eigenstates and eigenvalues are periodic in the reciprocal space with two periods which are multiples of one another.

We define dispersion curves so that the corresponding eigenstates $|\psi_{\mathbf{k},g}\rangle$ are continuous functions of \mathbf{k} over the extended Brillouin zone defined by the generalized translations, and g is the curve number. As an example, one of the curves is

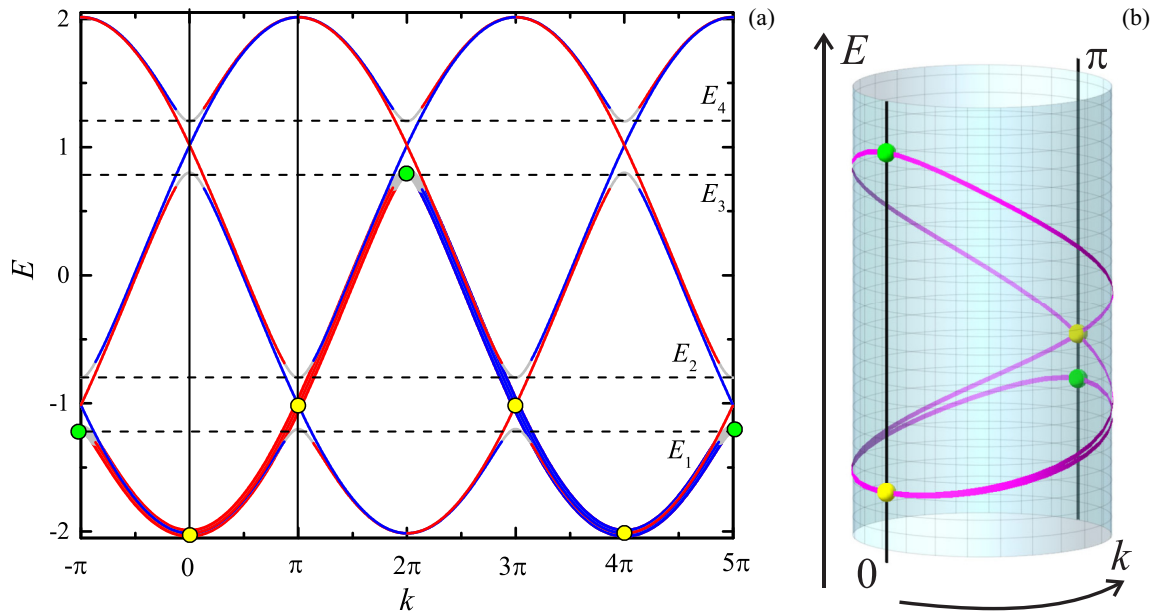


FIG. 1. (a) The electron band structure of the 1D model Eq. (10) and (b) a schematic cylindrical representation of the bottom dispersion curve, which is shown by the thick line in (a). The average spin along the curves is indicated by color: red and blue if $|\langle \hat{\sigma}_z \rangle| > 1/2$, gray otherwise. The yellow and green circles denote the degenerate and nondegenerate points, correspondingly.

shown in Fig. 1 by the thick line. According to the Bloch theorem, the eigenvalues should obey the conditions $\epsilon_{l, \mathbf{k}+\mathbf{K}} = \epsilon_{l, \mathbf{k}}$ where \mathbf{K} is the primitive vector of the magnetic reciprocal lattice and l is the eigenvalue number. One can see in Fig. 1 that a dispersion curve is not necessarily periodic in the magnetic Brillouin zone. However, the whole band structure has to be periodic to fulfill the Bloch theorem.

For instance, let us denote the lowest dispersion curve in the range from $-\pi$ to 0 in Fig. 1 by $|\psi_{\mathbf{k},1}\rangle$. It corresponds to $l = 1$ (eigenvalues indexed from the bottom to the top). However, while crossing $k = 0$ and, then, $k = \pi$, the eigenvalue number of the curve is changed by $l = 2$ and $l = 3$. That is, there is no a single-valued correspondence between g and l .

This leads to a nontrivial topology of dispersion curves. The curve marked by the thick line in Fig. 1(a) is schematically shown in a cylinder representation in Fig. 1(b). Paths on a cylinder can be classified by means of the fundamental group of cylinders [36]. The winding number coincides with n defined above and is a topological index. In the magnetic Brillouin zone, the band is reduced to n branches ($n = 3$ in Fig. 1). If the Fermi level falls into a gap between E_2 and E_1 (or between E_4 and E_3), an electron transport becomes unusual. A backward scattering without a spin flip is forbidden. There also exists a persistent spin current.

An additional uniform magnetic field directed along the spin z axis breaks the Kramers-like symmetry defined by Theorem 2. On the other hand, the Hamiltonian remains invariant under both translations. That is why the topological structure in Fig. 1(b) survives under the perturbation. A uniform magnetic field perpendicular to the z axis breaks both the Kramers-like symmetry and invariance under the generalized translations. In this case, the topology becomes trivial due to hybridization at the band crossing points.

The proved theorems and topological arguments can be applied to multidimensional systems. The conductive

hexagonal palladium layers in PdCrO_2 are described well by a 2D nearly-free-electron model [37]. Magnetic spacers CrO_2 form an effective field corresponding to a 120° (three-sublattice) magnetic structure [10]. Then, a solution for the Bloch wave functions ψ can be obtained from the following equation [35],

$$\left[\frac{\hbar^2}{2m} (\mathbf{k} - \mathbf{K})^2 - \mathcal{E} \right] \hat{c}_{\mathbf{k}-\mathbf{K}} + \sum_{\mathbf{K}'} \hat{U}_{\mathbf{K}'-\mathbf{K}} \hat{c}_{\mathbf{k}-\mathbf{K}'} = \mathbf{0}, \quad (11)$$

where \mathbf{k} is the wave vector within the magnetic Brillouin zone ($\sqrt{3} \times \sqrt{3}$), $\hat{U}_{\mathbf{K}}$ are the Fourier coefficients of effective field, and $\hat{c}_{\mathbf{k}}$ and $\hat{U}_{\mathbf{K}}$ have a spinor form [21]. In the case of a 2D system, the second term in Eq. (11) should contain at least two terms to describe properly the band structure in the vicinity of the K points (see Fig. 2).

Since the model Eq. (11) does not contain a spin-orbit coupling, the spin rotation axis z can be chosen to be arbitrary, and for the sake of simplicity, we direct it along the spatial z' axis, i.e., perpendicular to the plane. The Fourier coefficients have a special form in the case of a helical 120° effective field [21], $\hat{U}_{\mathbf{K}_{(z)}} = \gamma h_0 (\hat{\sigma}_x \pm i \hat{\sigma}_y)$, where γ is a complex coefficient. It should be mentioned that the spinor Fourier coefficients are abnormal operators [21].

The dispersion of the 2D model and the Fermi surface for two positions of the Fermi level are shown in Fig. 2. The topology of the dispersion surface is nontrivial. The volume of the extended Brillouin zone is three times larger than that of the magnetic one, therefore the topological index is $n = 3$. That is, if we close the periodic boundaries of the 2D magnetic Brillouin zone in a torus representation, the dispersion surface wrapping the torus contains three sheets. Intersections of the sheets occur along the Brillouin zone boundaries and along the Γ - K lines.

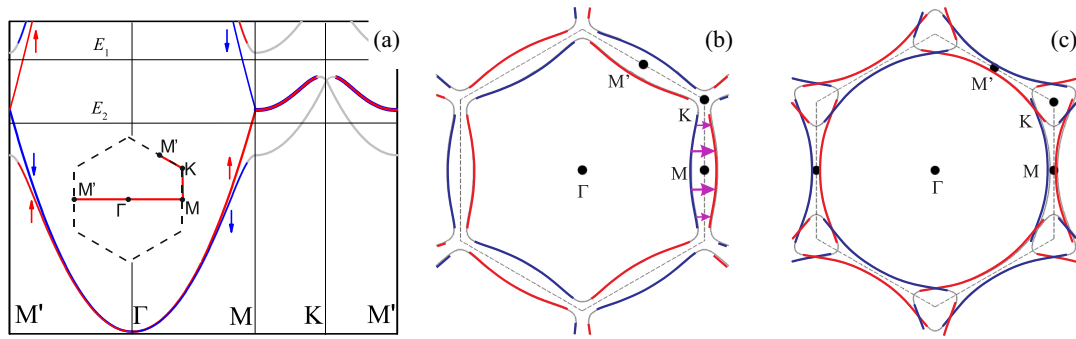


FIG. 2. (a) The dispersion of nearly-free-electron model Eq. (11) along the path shown in the inset, and the Fermi surface corresponding to the Fermi level positions at (b) E_1 and (c) E_2 . The average spin is indicated by color as in Fig. 1. The arrows in (b) schematically show umklapp scattering vectors.

Since the model satisfies Theorem 2 we again obtain relation (2). In Figs. 2(b) and 2(c), one can see that the opposite arcs of the Fermi surface are predominantly formed by opposite spins. This is an important result because this spin texture suppresses backward non-spin-flip scattering and umklapp electron-phonon scattering [21]. The arrows in Fig. 2(b) show transitions between initial and final electron states in the umklapp processes which are suppressed by the spin texture of the Fermi surface. Since at low temperatures an electron-phonon part of the resistance in metals with a closed Fermi surface is determined by umklapp scattering [38], the resistance is strongly suppressed [21] and a high-conductivity state appears.

In Fig. 2(c) one can see that pockets about the K points appear. This structure of the Fermi surface is similar to that which was observed experimentally in PdCrO_2 in a magnetically ordered state [14].

In conclusion, the two theorems proved above show that a Kramers-like degeneracy exists in a helical magnetic field. The topology of the band structure in helical magnetic systems is nontrivial. The traditional topological band theory developed for topological insulators deals with a phase of the wave function and its variation over the Brillouin zone. In the present Letter, the nontrivial topology stems from the fact

that commensurate helical systems have to be simultaneously periodic on the ordinary and generalized translations. This leads to a multisheet dispersion of electrons. The specific Kramers-like symmetry and topology lead to the spin texture of the Fermi surface, which suppresses the backward non-spin-flip scattering and umklapp electron-phonon scattering. As a result, a high-conductivity state appears. This effect is pronounced if a single band crosses the Fermi level (strong topological metal) because otherwise it is masked by interband scattering. This behavior is similar to that of topological surface and edge states in topological insulators [25]. However, in the present Letter we dealt with bulk states. The magnetic metallic delafossite PdCrO_2 is a candidate for a topological metal of this type. It should be mentioned that the band structure in Fig. 2 can also reproduce the nonreciprocity of electron transport under the magnetic field observed in this substance [2]. The effect discussed in the present Letter can be verified by noncollinear calculations within the density functional theory and spin-resolved angle-resolved photoelectron spectroscopy.

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