

On a New Type of Massless Dirac Fermions in Crystalline Topological Insulators[¶]

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A new type of massless Dirac fermions in *crystalline* three-dimensional topological insulators (three-dimensional \rightarrow two-dimensional situation) has been predicted. The spectrum has fourfold degeneracy at the top of the two-dimensional Brillouin zone (M point) and twofold degeneracy near the M point. Crystal symmetry along with the time reversal invariance in three-dimensional topological insulators allows fourfold degenerate Dirac cones, which are absent in the classification of topological features in R.-J. Slager et al., *Nat. Phys.* **9**, 98 (2013). The Hamiltonian in the cited work does not contain Dirac singularities with more than twofold degeneracy. For this reason, the corresponding topological classification is incomplete. The longitudinal magnetic field in the spinless case holds the massless dispersion law of fermions and does not lift fourfold degeneracy. In the spinor case, the magnetic field lifts fourfold degeneracy, holding only twofold degeneracy, and results in the appearance of a band gap in the spectrum of fermions.

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INTRODUCTION

Algebraic topological methods are fruitfully applied to many problems from quantum field theory to condensed matter physics. Although the foundations of mathematical methods are common, the methods themselves can vary depending on the formulations of problems. We briefly mention frequently used approaches. For example, the problem of the classification of structural defects and determination of their stability is reduced to the analysis of the equivalence classes of homotopic maps of a certain standard manifold associated with the bypass of a defect to the space of the order parameter. The classification is reduced to the list of homotopy groups associated with such maps [1].

A number of works involve a topological classification in a momentum space [2] based on the calculation of the torsion group (which is isomorphic to the group of integers \mathcal{L}) at the bypass of a singular point of the spectrum.

The formulation of the problem for crystal insulators differs from those mentioned above and is mainly reduced to the following questions.

(i) What nontrivial features of the electron spectrum dictated by spatial symmetries and time reversal invariance are possible on the surface in these systems at the symmetric \mathbf{k} points of the Brillouin zone? They

should not be present in the systematic of the bulk spectrum (should be beyond the projections of bulk bands, see below).

(ii) Are these singularities stable under continuous deformations of the Hamiltonian of the system under which the Hamiltonian is invariant under spatial symmetry elements and time reversal and which do not close the gap in the projections of bulk bands? This leads to the so-called \mathcal{L}_2 classification different from the mentioned \mathcal{L} classification of torsions in the momentum space.

Until now, for *crystalline* three-dimensional \rightarrow two-dimensional, two-dimensional \rightarrow one-dimensional, and *pure* two-dimensional systems, the features of the spectrum with twofold degeneracy at the symmetric points of the Brillouin zone (conical, $\varepsilon \sim \pm|\mathbf{k}|$; square, $\varepsilon \sim \pm|\mathbf{k}|^2$; and cubic, $\varepsilon \sim |\mathbf{k}|^3$) were discussed. Conical features of the spectrum were detected experimentally in pure two-dimensional systems (graphene), as well as in three-dimensional \rightarrow two-dimensional systems (BiSb binary compounds and heteroboundaries between IV–VI and II–VI semiconductors with band inversion) and two-dimensional \rightarrow one-dimensional crystal systems (see references in [3, 4]).

A question arises of whether conical features exist in crystalline systems with a higher degree of degeneracy. The study of the possibility of the appearance and experimental detection of such features (if they are possible) in crystalline three-dimensional \rightarrow two-dimensional and

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pure two-dimensional systems is an interesting topical problem.

Surface (edge) states with the conic dispersion law and with more than twofold degeneracy are absent in two-dimensional \rightarrow one-dimensional systems [5, 6], because the groups of borders do not allow more than twofold degeneracy because of the poverty of symmetry elements [6].

The ideal situation would be if particular materials or compounds where a larger degree of degeneracy is possible could be presented. However, it is currently impossible. *Nevertheless, it is possible to present a crystal structure of a compound with a conical massless spectrum with fourfold degeneracy.*

This problem is solved in this work. Moreover, fourfold degeneracy of the conical spectrum turns out to be maximally allowable in three-dimensional \rightarrow two-dimensional systems.

FOURFOLD DEGENERATE MASSLESS DIRAC FERMIONS

A crystal structure where fermions with a fourfold degenerate spectrum at $|\mathbf{k}| = 0$ (the quasimomentum \mathbf{k} is measured from the symmetric M point) and with a twofold degenerate spectrum at $|\mathbf{k}| \neq 0$ appear at the corner of the Brillouin zone (M point, see figure) is given below. This type of fermions can appear in both the three-dimensional \rightarrow two-dimensional and two-dimensional cases.

LATTICE SYMMETRY ELEMENTS

An example of the crystal lattice is shown in the figure. This lattice has a nonsymmorphic symmetry space group: it contains nontrivial translations by a half-period. Planes of symmetry exist only in combination with nontrivial translations by a half-period. The symmetry elements are $\{e|\mathbf{R}\}$, $\{C_4|\mathbf{R}\}$, $\{C_4^3|\mathbf{R}\}$, $\{C_2|\mathbf{R}\}$, $\{\sigma_x|\mathbf{R} + \alpha\}$, $\{\sigma_y|\mathbf{R} + \alpha\}$, and $\{\sigma_{xy}|\mathbf{R} + \alpha\}$, where $\{\mathbf{R}\} = (a, a)$ and $\{\alpha\} = (a/2, a/2)$ are the translations by a period and half-period, respectively.

PROJECTIVE IRREDUCIBLE REPRESENTATIONS OF THE GROUP OF THE WAVE VECTOR

The degree of degeneracy of energy bands at a certain point of the Brillouin zone is determined by the dimension of the irreducible representation of the group of the wave vector $G_{\mathbf{k}}$ of this point \mathbf{k} . We are interested in the M point (see figure) at which a nontrivial fourfold degenerate massless Dirac spectrum appears.

The group of the wave vector has a normal divisor, which is the translation group. The factor group of the group of the wave vector is isomorphic to the point

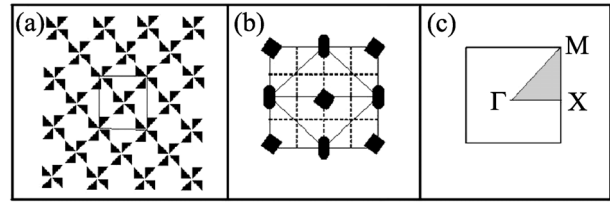


Fig. 1. (a) Example of the two-dimensional lattice with nontrivial translations [7]. (b) Lattice symmetry elements (the dashed lines are the sliding planes). (c) Irreducible part of the Brillouin zone.

group of directions $F_{\mathbf{k}}$. Since a space group contains nontrivial translations, projective representations inevitably appear. Let $\mathcal{D}(g)$ be the matrix of a certain representation of the space group and $\mathcal{D}^k(h)$ be the matrix of the representation of its factor group; for the symmetry element $g = \{h|\mathbf{R} + \alpha\} = \{h|\tau\}$ ($\tau = \mathbf{R} + \alpha$), they are related as $\mathcal{D}(g) = \exp(i\mathbf{k}\tau)\mathcal{D}^k(h)$. The product of the matrices of the representation for different elements of the group satisfies the law (see, e.g., [8])

$$\begin{aligned} \mathcal{D}(g_1)\mathcal{D}(g_2) &= \omega(g_1, g_2)\mathcal{D}(g_1 \cdot g_2), \\ \omega(g_1, g_2) &= e^{i(\mathbf{k} - \mathbf{g}_1^{-1}\mathbf{k})\alpha_2} = e^{i\mathbf{b}\alpha_2}, \end{aligned} \quad (1)$$

where $\mathbf{b} = \mathbf{k} - \mathbf{g}_1^{-1}\mathbf{k}$ is a certain reciprocal lattice vector. In our case, some factors $\omega(g_1 \cdot g_2)$ are not identically unity. Indeed,

$$\begin{aligned} \omega(C_4, \sigma_x) &= \exp[i(\mathbf{k} - C_4^{-1}\mathbf{k})\alpha] \\ &= \exp(2ik_y\alpha_x) = -1, \end{aligned} \quad (2)$$

$$\omega(\sigma_x, C_4) = \exp[i(\mathbf{k} - \sigma_x^{-1}\mathbf{k})0] = 1.$$

According to Eqs. (1) and (2), the representations of the group containing nontrivial translations are projective representations, rather than usual representations. The system of factors—the factor system $\omega(g_i \cdot g_j)$ —specifies projective representations of the group up to the factor $u(g)$ ($|u(g)| = 1$ is an arbitrary single-valued function on the elements of the group g). In this case, any two projective representations with the factor system from one class are related as $\mathcal{D}'(g) = \mathcal{D}(g)/u(g)$.

Different classes of factor systems are possible for one group. All factor systems from one class are related as $\omega'(g_1, g_2) = \omega(g_1, g_2)u(g_1g_2)/u(g_1)u(g_2)$. If all factors $\omega(g_1, g_2)$ can be made unity by the appropriate choice of $u(g)$, such a representation is equivalent to the usual vector representation of the group and belongs to the class K_0 . The factor system refers to a certain class according to the calculated factors ω for the generating elements of the point group. The point group C_{4v} under consideration has two generating elements: C_4 and σ_x ($(C_4)^4 = e$ and $(\sigma_x)^2 = e$). According to Eqs. (1) and (2), the factor system belongs to the class K_1 . This

Table

C_{4v}	e e	a, a^3 C_4, C_4^3	a^2 C_2	b, a^2b σ_x, σ_y	ab, a^3b σ_{xy}, σ_{yx}	Functions, tensor components
$P_1^{(1)}$	2	$i\sqrt{2}$	0	0	0	
$P_2^{(1)}$	2	$-i\sqrt{2}$	0	0	0	
E_1'	2	$\sqrt{2}, -\sqrt{2}$	0	0	0	$(\alpha\rangle, \beta\rangle)$
E_2'	2	$-\sqrt{2}, \sqrt{2}$	0	0	0	$((x+iy)\alpha\rangle, (x-iy)\beta\rangle)$
E	2	0	-2	0	0	$(x, y), (k_x, k_y), (H_y, -H_x)$

means that the representations of the group of the wave vector are not reduced to vector representations and are projective representations. All projective representations for point groups have long been constructed and were represented in, e.g., [8]. The group C_{4v} has two two-dimensional projective representations, $P_1^{(1)}$ and $P_2^{(1)}$, whose factor system belongs to the class K_1 (the factor system can be reduced to the standard form, but this is not required below).

The table presents the characters of two-dimensional projective ($P_1^{(1)}$ and $P_2^{(1)}$), spinor (E_1' and E_2'), and vector (E) representations, as well as wavefunctions and components of the wave vectors and magnetic field, which are transformed according to the spinor and vector representations, respectively. The spinor representations are not used below. They are presented to illustrate their genetic connection with projective representations to which they are transferred. The two-dimensionality of the representations means that the spectrum at the M point disregarding time reversal symmetry would be twofold degenerate both in the spinless case and in the spinor case.

REQUIREMENTS OF THE TIME REVERSAL INVARIANCE

The Hamiltonian under consideration is invariant not only under crystal symmetry operations but also under time reversal. This symmetry can result in additional degeneracy of the spectrum. Time reversal \mathcal{H} in the spinless case is reduced to the complex conjugation of the wavefunction $\mathcal{H}\psi = \psi^*$. In the presence of the spin-orbit interaction, the time reversal operator has the form $\mathcal{H}\psi = \sigma_y\psi^*$ and

$$\begin{aligned} & \mathcal{H}^2\psi = K^2\psi \\ & = \begin{cases} \sigma_y(\sigma_y\psi^*)^* = -\psi, & K^2 = -1 \text{ (spinor case),} \\ (\psi^*)^* = \psi, & K^2 = +1 \text{ (spinless case).} \end{cases} \quad (3) \end{aligned}$$

(The time reversal operator is also used in the equivalent form $\mathcal{H}\psi = i\sigma_y\psi^*$. The form of the representation of the time reversal operator depends on the choice of the spin-orbit interaction in the Hamiltonian with a factor with or without an imaginary unity.) Let the set of wavefunctions $\psi_{k,i}^\mu$ of a certain energy level be transformed according to the irreducible representation $\mathcal{D}_\mu^k(g)$ of the group of the wave vector G_k . Then, the set of wavefunctions related to $\psi_{k,i}^\mu$ through the time reversal operator $\mathcal{H}\psi_{k,i}^\mu$ is transformed according to the complex conjugate representation $\mathcal{D}_\mu^{k*}(g)$. Two situations are possible. In the first situation, the sets of functions $\psi_{k,i}^\mu$ and $\mathcal{H}\psi_{k,i}^\mu$ are linearly dependent (coincide up to a unitary rotation); i.e., they are expressed in terms of each other:

$$\mathcal{H}\psi_{k,i}^\mu = \sum_j T_{ij}\psi_{k,j}^\mu, \quad (4)$$

where T_{ij} is the matrix of the unitary operator. In this situation, the time reversal symmetry of the Hamiltonian *does not lead to additional degeneracy*. In the second situation, the sets of the functions $\psi_{k,i}^\mu$ and $\mathcal{H}\psi_{k,i}^\mu$ are linearly independent; i.e., they do not coincide with each other. In this case, the time reversal invariance results in an additional degeneracy of levels. Thus, there are three cases: (a) the functions $\psi_{k,i}^\mu$ and $\mathcal{H}\psi_{k,i}^\mu$ are linearly dependent, (b) the functions $\psi_{k,i}^\mu$ and $\mathcal{H}\psi_{k,i}^\mu$ are linearly independent and the representations $\mathcal{D}_\mu^k(g)$ and $\mathcal{D}_\mu^{k*}(g)$ are nonequivalent and have complex-valued characters, and (c) the functions $\psi_{k,i}^\mu$ and $\mathcal{H}\psi_{k,i}^\mu$ are linearly independent and the representations $\mathcal{D}_\mu^k(g)$ and $\mathcal{D}_\mu^{k*}(g)$ are equivalent and have real-valued characters.

The case of fourfold degeneracy considered below refers to variant b_1 [8]. The subscript 1 means that all \mathbf{M} points are equivalent and appear in one star of the wave vector, whereas the representations $P_{1,2}^{(1,2)}$ are nonequivalent and have complex-valued characters. The Herring criterion [9] makes it possible to distinguish three cases

$$\Sigma = \frac{1}{h} \sum_{g \in G_k^i} \chi_k(g^2) \delta_{k, -gk} = \begin{cases} K^2 & (\text{case } a), \\ 0 & (\text{case } b), \\ -K^2 & (\text{case } c), \end{cases} \quad (5)$$

where summation is performed over the elements of the group of the wave vector for which $g\mathbf{k} = -\mathbf{k}$. We now calculate this sum. Let the matrices of the projective representations for the generating symmetry elements be $a \equiv C_4 - \mathbf{A}$ and $b \equiv \sigma_x - \mathbf{B}$ and satisfy the relations $\mathbf{A}^4 = -\mathbf{I}$, $\mathbf{B}^2 = \mathbf{I}$, and $\mathbf{B}\mathbf{A} = \mathbf{A}^3\mathbf{B}$, where \mathbf{I} is the 2×2 identity matrix and $(ab)^2 = abab = a(a^3b)b = a^4b^2$. Using the characters for the representation $P_{1,2}^{(1,2)}$,

$$\begin{aligned} \Sigma &= \chi(e^2) + 2\chi[(C_4)^2] + \chi[(C_2)^2] + 2\chi[(\sigma_x)^2] \\ &+ 2\chi[(\sigma_{xy})^2] = \chi(e^2) + 2\chi(a^2) + \chi(a^4) + 2\chi(b^2) \\ &+ 2\chi(abab) = \text{Tr}[\mathbf{I} + 2\mathbf{A}^2 + 2\mathbf{B}^2 + 2\mathbf{A}^4\mathbf{B}^2] \\ &= 2 + 2 \cdot 0 - 2 + 2 \cdot 2 - 2 \cdot 2 = 0, \end{aligned} \quad (6)$$

we find that the doubling of the dimension of representations and additional degeneracy owing to time reversal appear both disregarding the spin and taking into account the spin-orbit interaction.

HAMILTONIAN OF THE SYSTEM

To construct the Hamiltonian near the \mathbf{M} point, it is convenient to use the invariant method [8]. Let $\mathcal{D}(g)$ be a certain representation of the group of the spatial symmetry of the crystal at the \mathbf{k} point and $\hat{\mathbf{H}}(k)$ be the Hamiltonian. The invariance of the Hamiltonian with respect to the symmetry element g means that

$$\hat{\mathbf{H}}'(k') = \mathcal{D}(g)\hat{\mathbf{H}}(g^{-1}k)\mathcal{D}^{-1}(g) = \hat{\mathbf{H}}(k). \quad (7)$$

The Hamiltonian matrix $\hat{\mathbf{H}}(k)$ can be represented in terms of the product of the tensors (powers of the components of the wave vector, components of the magnetic field, and other physical quantities) k_i^κ and certain basis matrices $\hat{\mathbf{X}}_i$, which, taking into account Eq. (7), are transformed as

$$\begin{aligned} g^{-1}\hat{\mathbf{X}}_i &= \hat{\mathbf{X}}'_i = \mathcal{D}(g)\hat{\mathbf{X}}_i\mathcal{D}^{-1}(g), \\ \hat{\mathbf{X}}'_i &= \sum_j \mathcal{D}_{ij}^X(g)\hat{\mathbf{X}}_j. \end{aligned} \quad (8)$$

Consequently, a set of basis matrices can always be chosen so (for details, see [8]) that the representation $\mathcal{D}^X(g)$ according to which matrices in Eqs. (7) and (8) transform is the direct product $\mathcal{D}(g)\mathcal{D}^*(g)$ of matrices in Eqs. (8).

The tensor components k_i^κ transform according to the usual irreducible vector representations $\mathcal{D}_\kappa(g)$ of the groups of directions F_k of the \mathbf{k} point. The representation $\mathcal{D}^X(g)$ has the characters $\chi^X(g) = |\chi(g)|^2$ and is generally irreducible in the group F_k (representation $\mathcal{D}(g)$ is a certain irreducible representation $\mathcal{D}_\mu^k(g)$ of the group of the wave vector G^k at the \mathbf{k} point, see below). This representation can be expanded into irreducible representations. Let $\hat{\mathbf{X}}_i^\kappa$ be a set of matrices transformed according to the κ th irreducible representation F_k (the subscript i means that several different sets of matrices can exist). Further, let $k_i^{\kappa*}$ be the tensor components transformed according to the irreducible representation $\mathcal{D}_\kappa^*(g)$ conjugate to F_k . Then, the Hamiltonian can include invariant terms transformed according to the identity representation:

$$\hat{\mathbf{H}}(k) = \sum_i d_i \hat{\mathbf{X}}_i^\kappa k_i^{\kappa*}, \quad (9)$$

where d_i are the material constants, which can be taken real under the condition that the matrices $\hat{\mathbf{X}}_i^\kappa$ are chosen Hermitian [8]. The number of independent terms with the superscript κ in Eq. (9) is determined by the number of appearance of the representation $\mathcal{D}_\kappa(g)$ in the representation $\mathcal{D}^X(g)$ (see Eqs. (13) and (14)).

UNIFICATION OF REPRESENTATIONS AT TIME REVERSAL

Since time reversal requires the integration of two projective representations, the basis $\psi_I, \psi_{II} = \mathcal{K}\psi_I$ should be used to construct the corresponding Hamiltonian. The functions are transformed according to the representations D_μ^k and $D_\mu^{\kappa*}$, respectively. The functions are transformed to each other by the operator

$$\hat{\mathbf{T}} = \begin{pmatrix} 0 & \mathcal{K}^2\mathbf{I} \\ \mathbf{I} & 0 \end{pmatrix}. \quad (10)$$

The time reversal invariance of the Hamiltonian in the basis ψ_I, ψ_{II} means that

$$\begin{aligned} \hat{\mathbf{T}}^{-1}\hat{\mathbf{H}}(fk)\hat{\mathbf{T}} &= \hat{\mathbf{H}}(k)^*, \\ \hat{\mathbf{H}}(k) &= \begin{pmatrix} \mathbf{H}_{II}(k) & \mathbf{H}_{I\ II}(k) \\ \mathbf{H}_{I\ I}(k) & \mathbf{H}_{II}(k) \end{pmatrix}. \end{aligned} \quad (11)$$

Conditions (11) imply constraints on the diagonal and off-diagonal matrix elements of the Hamiltonian:

$$\mathbf{H}_{\Pi\Pi}(k) = \mathbf{H}_{\Pi\Pi}^*(fk), \quad \mathbf{H}_{\Pi I}(k) = K^2 \mathbf{H}_{I\Pi}^*(fk), \quad (12)$$

where $f = +$ and $-$ for even and odd tensor components k_i^κ under time reversal. It remains only to calculate the number of independent sets of basis matrices. The number of independent sets with the index κ for the diagonal matrix elements is determined by the number of appearance of the product of the representations $\mathcal{D}_\mu(g)^{\kappa} \mathcal{D}_\mu(g)^{\kappa*}$ in the representation $\mathcal{D}_\kappa(g)$; i.e.,

$$N_{\text{diag}} = \frac{1}{h} \sum_{g \in G_k^*} |\chi_\mu^k(g)|^2 \chi_\kappa(g). \quad (13)$$

Similarly, the number of independent off-diagonal sets of matrices is determined from the condition [8]

$$N_{\text{off-diag}} = \frac{1}{2h} \sum_{g \in G_k^*} \chi_\kappa(g) \{ [\chi_\mu^k(g)]^2 + K^2 f \chi_\mu^k(g^2) \}, \quad (14)$$

where $\chi_\mu^k(g)$ is the character of the representation of the group of the wave vector G_k ($P_{1,2}^{(1,2)}$) of the k point and $\chi^\kappa(g)$ is the character of the representation of the point group of directions F_k . The number of independent diagonal matrices

$$N_{\text{diag}} = \frac{1}{8} [|\chi_\mu^k(e)|^2 + 2\chi_\kappa(C_4) |\chi_\mu^k(C_4)|^2 + \chi_\kappa(C_2) |\chi_\mu^k(C_2)|^2 + 2\chi_\kappa(\sigma_x) |\chi_\mu^k(\sigma_x)|^2 + 2\chi_\kappa(\sigma_{xy}) |\chi_\mu^k(\sigma_{xy})|^2] \quad (15)$$

$$= \frac{1}{8} [2 \cdot 2^2 + 2 \cdot 0 \cdot 2 - 2 \cdot 0 \cdot 0 + 2 \cdot 0 \cdot 0] = 1;$$

for both projective representations of the group of the wave vector G_k , $\mathcal{D}_\mu^k \rightarrow P_1^{(1)}$ and $\mathcal{D}_\mu^{k*} \rightarrow P_2^{(2)}$.

One of the sets of matrices transformed similar to (k_x, k_y) can be taken in the form

$$(\mathbf{X}_x, \mathbf{X}_y) = \left(\left(\begin{array}{cc} \sigma_y & 0 \\ 0 & \sigma_y \end{array} \right)_x, \left(\begin{array}{cc} -\sigma_x & 0 \\ 0 & \sigma_x \end{array} \right)_y \right). \quad (16)$$

The last matrices satisfy the relations for diagonal components of Hamiltonian (12) and are odd in time. The Hamiltonian in *both spinless and spinor cases* has the term $\mathcal{H}(\mathbf{k}) \sim d(\mathbf{X}_x k_x + \mathbf{X}_y k_y)$, where d is *one common material constant*.

The number of independent off-diagonal sets of the basis matrices of the Hamiltonian given by Eq. (14) can be calculated similar to Eqs. (13) and (15). The numbers of off-diagonal sets are different in the spinless and spinor cases because of the factor K^2 in Eq. (14) ($K^2 = 1$ and -1 in the spinless and spinor cases, respectively). The number of off-diagonal sets is $N_{\text{off-}}$

$\text{diag} = 0$ for the spinless case and is $N_{\text{off-diag}} = 2$ for the spinor case. It is convenient to choose the following two sets, which naturally satisfy Eqs. (12) dictated by the time reversal invariance:

$$(\mathbf{X}_x^{(1)}, \mathbf{X}_y^{(1)}) = \left(\left(\begin{array}{cc} 0 & -i\sigma_x \\ i\sigma_x & 0 \end{array} \right)_x, \left(\begin{array}{cc} 0 & -\sigma_x \\ -\sigma_x & 0 \end{array} \right)_y \right) \quad (17)$$

$$(\mathbf{X}_x^{(2)}, \mathbf{X}_y^{(2)}) = \left(\left(\begin{array}{cc} 0 & -i\sigma_z \\ i\sigma_z & 0 \end{array} \right)_x, \left(\begin{array}{cc} 0 & -\sigma_z \\ -\sigma_z & 0 \end{array} \right)_y \right).$$

SPECTRUM OF FERMIONS

The final forms of the Hamiltonian and spectrum are as follows.

In the spinless case,

$$\begin{aligned} \mathcal{H}(\mathbf{k}) &= d(\mathbf{X}_x k_x + \mathbf{X}_y k_y), \\ \varepsilon_1^\pm(\mathbf{k}) &= \pm v|\mathbf{k}|, \\ \varepsilon_2^\pm(\mathbf{k}) &= \pm v|\mathbf{k}|, \quad v = |d|. \end{aligned} \quad (18)$$

The spectrum of quasiparticles has a massless dispersion law and is fourfold degenerate at $\mathbf{k} = 0$ and twofold degenerate at $\mathbf{k} \neq 0$ ($\mathbf{k} = (k_x, k_y)$).

In the spinor case,

$$\begin{aligned} \mathcal{H}(\mathbf{k}) &= d(\mathbf{X}_x k_x + \mathbf{X}_y k_y) \\ &+ d_1(\mathbf{X}_x^{(1)} k_x + \mathbf{X}_y^{(1)} k_y) + d_2(\mathbf{X}_x^{(2)} k_x + \mathbf{X}_y^{(2)} k_y). \end{aligned} \quad (19)$$

The diagonalization of Eq. (19) gives the spectrum of fermions:

$$\begin{aligned} \varepsilon_1^\pm(\mathbf{k}) &= \mp v_s |\mathbf{k}|, \quad \varepsilon_2^\pm(\mathbf{k}) = \pm v_s |\mathbf{k}|, \\ v_s &= \sqrt{d^2 + d_1^2 + d_2^2}. \end{aligned} \quad (20)$$

SPECTRUM IN THE LONGITUDINAL MAGNETIC FIELD

The longitudinal magnetic field in the two-dimensional structure does not result in quantization. The components of the magnetic field appear in the Hamiltonian with their material constants. The number of independent sets of diagonal and off-diagonal sets of matrices is determined similar to the preceding case with the components of the wave vector. Taking into account the table, we arrive at the following conclusions.

In the spinless case, the Hamiltonian and spectrum in the longitudinal field $\mathbf{H} = (H_y, -H_x)$ have the form

$$\begin{aligned} \mathcal{H}(\mathbf{H}) &= Q(\mathbf{X}_x H_y - \mathbf{X}_y H_x), \\ \varepsilon_1^\pm(\mathbf{k}, \mathbf{H}) &= \pm v|\mathbf{k} + q\mathbf{H}|, \\ \varepsilon_2^\pm(\mathbf{k}, \mathbf{H}) &= \pm v|\mathbf{k} + q\mathbf{H}|, \quad q = Q/d. \end{aligned} \quad (21)$$

where Q is a common material constant. The spectrum of quasiparticles has a massless dispersion law, is fourfold degenerate at $\mathbf{k} = -q\mathbf{H}$, and twofold degenerate at $\mathbf{k} \neq -q\mathbf{H}$. The magnetic field leads to the shift of the origin in \mathbf{k} . The longitudinal magnetic field results in the change

$$k_x \longrightarrow k_x + qH_y, \quad k_y \longrightarrow k_y - qH_x. \quad (22)$$

In the spinor case, the Hamiltonian and spectrum in the longitudinal field $\mathbf{H} = (H_y, -H_x)$ have the form

$$\begin{aligned} \mathcal{H}(\mathbf{H}) &= Q(\mathbf{X}_x H_y - \mathbf{X}_y H_x) \\ &+ Q_1(\mathbf{X}_x^{(1)} H_y - \mathbf{X}_y^{(1)} H_x) \\ &+ Q_2(\mathbf{X}_x^{(2)} H_y - \mathbf{X}_y^{(2)} H_x). \end{aligned}$$

$$\begin{aligned} \varepsilon_1^\pm(\mathbf{k}, \mathbf{H}) &= \pm \sqrt{d^2(\mathbf{k} + q\mathbf{H})^2 + d_1^2(\mathbf{k} + q_1\mathbf{H})^2 + d_2^2(\mathbf{k} + q_2\mathbf{H})^2}, \\ \varepsilon_2^\pm(\mathbf{k}, \mathbf{H}) &= \pm \sqrt{d^2(\mathbf{k} + q\mathbf{H})^2 + d_1^2(\mathbf{k} + q_1\mathbf{H})^2 + d_2^2(\mathbf{k} + q_2\mathbf{H})^2}, \\ q &= Q/d, \quad q_{1,2} = Q_{1,2}/d_{1,2}. \end{aligned}$$

where Q , Q_1 , and Q_2 are the material constants. The magnetic field in the spinor case leads to the change in the components of the wave vector similar to Eq. (22), but with different material constants. As a result, a gap opens between the positive and negative branches of the spectrum. In this case, only twofold degeneracy remains. At high values $|\mathbf{k}| \gg \{q, q_{1,2}|\mathbf{H}\}$, the spectrum approaches the twofold degenerate cone given by Eqs. (20).

INTERPRETATION OF THE RESULTS

Time reversal disregarding the spin-orbit interaction provides the unification of two-dimensional representations with the same constant d for both representations. In the first representation (see table), the basis is a pair of functions genetically occurring from the states $|\alpha\rangle = |1/2\rangle$ and $|\beta\rangle = |-1/2\rangle$; in the second representation, a pair of functions genetically occurring from the states $|(x + iy)\alpha\rangle = |3/2\rangle$ and $|(x - iy)\beta\rangle = |-3/2\rangle$. Here, $|\pm 1/2, \pm 3/2\rangle$ are the functions with certain projections of the pseudomomentum. The degenerate branches of the spectrum correspond to the

$$\begin{aligned} \text{wavefunctions } |\Psi_1^\pm\rangle &= \frac{1}{\sqrt{2}} \left(e^{i\varphi(\mathbf{k})/2} \left| \frac{1}{2} \right\rangle \pm e^{-i\varphi(\mathbf{k})/2} \left| -\frac{1}{2} \right\rangle \right) \\ \text{and } |\Psi_2^\pm\rangle &= \frac{1}{\sqrt{2}} \left(e^{i\varphi(\mathbf{k})/2} \left| \frac{3}{2} \right\rangle \pm e^{-i\varphi(\mathbf{k})/2} \left| -\frac{3}{2} \right\rangle \right), \text{ where} \end{aligned}$$

$$\varphi(\mathbf{k}) = \arg \frac{ik_x + k_y}{\sqrt{k_x^2 + k_y^2}}.$$

In the longitudinal magnetic field, fourfold degeneracy is not lifted in the spinless case. The field results only in the shift of the vertex of the cone from the point $\mathbf{k} = 0$ to the point $\mathbf{k} = -q\mathbf{H}$ (21).

When the spin-orbit interaction is taken into account, there are three independent constants q , q_1 , and q_2 . In this case, the wavefunction that is a superposition of all four functions with different projections of the pseudomomentum $|\Psi_i^\pm\rangle = c_{i,1/2}^\pm \left| \frac{1}{2} \right\rangle + c_{i,1/2}^\pm \left| -\frac{1}{2} \right\rangle +$

$$c_{i,3/2}^\pm \left| \frac{3}{2} \right\rangle + c_{i,-3/2}^\pm \left| -\frac{3}{2} \right\rangle, \text{ where } i = 1, 2, \text{ corresponds to}$$

each branch of the spectrum. In the longitudinal magnetic field in the spinor case, fourfold degeneracy is changed to twofold degeneracy. The magnetic field opens a gap in the spectrum. This is physically due to the fact that the magnetic field breaks time reversal invariance and destroys the ‘‘unification’’ of complex conjugate representations in the spinor case. When the spin is disregarded, the unification of complex conjugate representations is trivial in a certain sense, because the Hamiltonian matrix has the block diagonal form given by Eq. (18). The magnetic field acts identically on each block, holding degeneracy.

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