Spin-orbit coupling and semiclassical electron dynamics in noncentrosymmetric metals

K. V. Samokhin∗

Department of Physics, Brock University, St. Catharines, Ontario L2S 3A1, Canada

Spin-orbit coupling of electrons with the crystal lattice plays a crucial role in materials without inversion symmetry, lifting spin degeneracy of the Bloch states and endowing the resulting nondegenerate bands with complex spin textures and topologically nontrivial wavefunctions. We present a detailed symmetry-based analysis of the spin-orbit coupling and the band degeneracies in noncentrosymmetric metals. We systematically derive the semiclassical equations of motion for fermionic quasiparticles near the Fermi surface, taking into account both the spin-orbit coupling and the Zeeman interaction with an applied magnetic field. Some of the lowest-order quantum corrections to the equations of motions can be expressed in terms of a fictitious “magnetic field” in the momentum space, which is related to the Berry curvature of the band wavefunctions. The band degeneracy points or lines serve as sources of a topologically nontrivial Berry curvature. We discuss the observable effects of the wavefunction topology, focusing, in particular, on the modifications to the Lifshitz-Onsager semiclassical quantization condition and the de Haas-van Alphen effect in noncentrosymmetric metals.

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∗ E-mail: kirill.samokhin@brocku.ca
I. INTRODUCTION

Majority of metals have a center of inversion in their crystal lattice. Recently, however, there has been growing interest, both experimental and theoretical, in the properties of noncentrosymmetric metals, driven mostly by their unusual properties in the superconducting state. Starting from the discovery of superconductivity in a heavy-fermion compound CePt$_3$Si (Ref. 1), the list of noncentrosymmetric superconductors has been steadily growing and now includes dozens of materials, such as UIr (Ref. 2), CeRhSi$_3$ (Ref. 3), CeIrSi$_3$ (Ref. 4), Y$_2$C$_3$ (Ref. 5), Li$_2$(Pd$_{1-x}$Pt$_x$)$_3$B (Ref. 6), KOs$_2$O$_6$ (Ref. 7), and many others. What sets crystals without inversion symmetry apart from their centrosymmetric counterparts (which are the ones usually considered in the literature) is the role of the spin-orbit (SO) coupling of electrons with the lattice potential. In contrast to the centrosymmetric case, it qualitatively changes the nature of the electron wavefunctions, lifting the spin degeneracy of the Bloch bands almost everywhere in the Brillouin zone, and resulting in a complex spin texture of the bands in the momentum space. This has profound consequences for superconductivity, including unusual nonuniform ("helical") superconducting phases,[8, 9, 10, 11, 12] magnetolectric effect,[13, 14, 15, 16] and a strongly anisotropic spin susceptibility with a large residual component.[14, 17, 18, 19, 20]

One subject that has received little attention in the recent studies of noncentrosymmetric metals is the effects of the spin texture and the wavefunction topology in the normal state. Topological properties of wavefunctions are known to play a crucial role in many condensed matter systems. A classic example is the integer quantum Hall effect, which was explained in Ref. 21 in terms of the Chern numbers of the magnetic Bloch bands, see also Ref. 22. Other examples include the spontaneous (anomalous) Hall effect in ferromagnetic metals and semiconductors, whose relation to the wavefunction topology was emphasized in Refs. 23, 24, 25, the spin Hall effect,26, 27 the quantum spin Hall effect in topological band insulators,28, 29, 30 and electric polarization of crystalline insulators.31

One common feature shared by these systems is the importance of the Berry phase of band electrons. Discovered originally in the context of quantum systems with adiabatically changing parameters,32 the Berry phase found its applications in many areas of physics, see, e.g., Ref. 33, and was introduced into the dynamics of electrons in solids in Ref. 34. For Bloch electrons, the role of the parameter space is played by the reciprocal (or momentum)
space: If, when subjected to a slowly varying external field, the quasiparticle wave vector evolves semiclassically along a closed path in the Brillouin zone, then the wavefunction picks up a path-dependent Berry phase. It is the Berry phase, or, more precisely, the flux of the associated Berry curvature through the magnetic Brillouin zone in two dimensions, that determines the quantized Hall conductivity.\[21\] Nonzero Berry curvature also determines the lowest-order quantum corrections to the semiclassical dynamics of quasiparticles, leading, in particular, to anomalous velocity terms in the equations of motions. While the importance of such terms was noticed several decades ago,\[35\] their relation to the topological characteristics of the band wavefunctions was established only recently, see Refs. 36, 37.

Among the effects of the anomalous velocity that are of particular relevance to metals is the modification of the Lifshitz-Onsager relation, which describes the semiclassical quantization of the electron energy levels in an applied magnetic field: \[A(E) = (2\pi \hbar eB/c)(n + \gamma)\] (Ref. 38). Here \(B\) is the magnetic field, \(A\) is the cross-sectional area of a closed classical orbit of an electron in momentum space, and \(n\) is a large positive integer. As for the correction \(\gamma\), while it is common to use \(\gamma = 1/2\), it is no longer the case if the electron spin and the SO coupling are taken into account. This was analyzed in detail for a centrosymmetric metal in Ref. 39, and revisited recently in Refs. 40, 41, where it was shown that \(\gamma\) has a non-universal value, which depends on the details of the orbit.

The goal of this paper is twofold. First, we want to present a systematic analysis of the SO coupling of band electrons in noncentrosymmetric crystals, which is done in Sec. 11. Sec. 11A focuses on the role of point-group and time-reversal symmetries in determining the structure of the SO coupling in the reciprocal space. In Sec. 11B we define the basis of Bloch pseudospin eigenstates and discuss the distinction between the symmetric and antisymmetric SO coupling, the latter being nonzero only in the noncentrosymmetric case. In Sec. 11C we introduce the generalized Rashba model and provide explicit expressions for the antisymmetric SO coupling for all noncentrosymmetric crystal symmetries. A distinctive feature of noncentrosymmetric crystals is that the antisymmetric SO coupling always vanishes, for symmetry reasons, at some isolated points or even whole lines in the Brillouin zone, which leads to the presence of mandatory band degeneracies, see Sec. 11D.

Our second goal is to derive the semiclassical equations of motion of fermionic quasiparticles in noncentrosymmetric metals, which is done in Sec. 11I. The spin effects play a crucial role and need to be fully taken into account: In addition to the interaction with an exter-
nal magnetic field, we include the antisymmetric SO coupling of electron with the crystal lattice potential, as well the effects of the exchange field in a magnetic crystal. We consider only the case of noninteracting electrons. We assume that the band splitting caused by the SO coupling is sufficiently strong to make it possible to treat the quasiparticle dynamics in different nondegenerate bands independently. The semiclassical equations of motion can be derived using various techniques, see, e.g., the wave-packet Lagrangian formalism of Ref. [37]. Our derivation in Sec. IIIA, which is based on the general semiclassical analysis for multicomponent wavefunctions developed by Littlejohn and Flynn,[42] yields the semiclassical Hamiltonian and the equations of motions containing terms of the zeroth as well as the first order in Planck’s constant $\hbar$. The latter can be dubbed “quantum corrections”, and are shown to depend on the Berry curvature of the SO split bands. In Sec. III B the contributions of the band degeneracy points and lines to the Berry curvature are discussed.

Finally, in Sec. IV we apply the theory developed in the preceding sections to the Lifshitz-Onsager quantization and the de Haas-van Alphen (dHvA) effect in noncentrosymmetric metals (Sec. IV A), and also to the anomalous Hall effect (AHE) in ferromagnetic noncentrosymmetric metals (Sec. IV B).

II. SPIN-ORBIT COUPLING IN NONCENTROSYMMETRIC CRYSTALS

Our starting point is the following Hamiltonian for non-interacting electrons in a crystal:

$$\hat{H} = \frac{\hat{p}^2}{2m} + U(r) + \frac{\hbar}{4me^2}\vec{\sigma}[\nabla U(r) \times \hat{p}],$$

(1)

where $\hat{p} = -i\hbar\nabla$ is the momentum operator, $U(r)$ is the crystal lattice potential, and $\vec{\sigma}$ are the Pauli matrices. We neglect impurities, lattice defects, and phonons, so that $U(r)$ has the perfect periodicity of a Bravais lattice. In the absence of the SO coupling, which is described by the last term, $\hat{H}_{SO}$, the eigenstates of the Hamiltonian are the Bloch spinors, labelled by the wave vector $k$ (which takes values in the first Brillouin zone), the band index $n$, and the spin index $s$:

$$\langle r\sigma|kns \rangle = \frac{1}{\sqrt{V}}\varphi_{kn}(r)e^{i\vec{k}\cdot\vec{r}}\chi_s(\sigma).$$

(2)

Here $V$ is the system volume, $\sigma = \uparrow, \downarrow$ is the spin projection, $\varphi_{kn}(r)$ have the same periodicity as the crystal lattice, and $\chi_s(\sigma)$ are the basis spinors: $\chi_s(\sigma) = \delta_{s\sigma}$. The corresponding eigenvalues have the following symmetry properties: $\epsilon_n(k) = \epsilon_n(-k)$, $\epsilon_n(k) = \epsilon_n(g^{-1}k)$,
where \( g \) is an operation from the point group of the crystal. We will call the electron bands calculated without the SO coupling the “orbital” bands.

Let us calculate the matrix elements of the electron-lattice SO coupling in the basis of the Bloch states (2):

\[
\langle kns | \hat{H}_{SO} | k'n's' \rangle = \frac{\hbar}{4m^2c^2} \sum_{ijl} e_{ijl} \langle s | \hat{\sigma}_i | s' \rangle \frac{1}{V} \int d^3r \Theta_{jl}(r) e^{i(k'-k)r},
\]

where \( i, j, l = x, y, z \), and

\[
\Theta_{jl}(r) = (\nabla_j U)(r)(\hat{p}_l + \hbar k_{l}')(\hat{p}_l + \hbar k_{l}).
\]

Since \( \Theta_{jl} \) are lattice-periodic functions of \( r \), the integral in Eq. (3) is nonzero only if \( k' - k = G \), where \( G \) is a reciprocal lattice vector. Because both \( k \) and \( k' \) are in the first Brillouin zone, the only possibility is \( k' = k \). The Hamiltonian remains nondiagonal in both the band and spin indices, and can be written in the second-quantized form as follows:

\[
H = \sum_k \sum_{n,n'} \sum_{s,s'} [\epsilon_n(k) \delta_{nn'} \delta_{ss'} + L_{nn'}(k) \sigma_{ss'}] a_{kn}^\dagger a_{kn'},
\]

where \( a^\dagger \) and \( a \) are the electron creation and annihilation operators, the chemical potential is included in the band dispersion functions (we neglect the difference between the chemical potential and the Fermi energy \( \epsilon_F \)), and the functions

\[
L_{nn'}(k) = \frac{\hbar}{4m^2c^2} \frac{1}{V} \int d^3r \nabla U(r) \times [\varphi^*_kn(r)(\hat{p} + \hbar k)\varphi_{kn'}(r)]
\]

decribe the SO coupling. The components of \( L_{nn'} \) with \( n = n' \) and \( n \neq n' \) can be interpreted, respectively, as the intraband and interband matrix elements of the orbital angular momentum of band electrons. The integration in Eq. (5) is performed over the unit cell of volume \( V \). The Hamiltonian (4) is exact for non-interacting electrons, regardless of the band structure and the strength of the SO coupling.

### A. Symmetry of the SO coupling

Although one can, in principle, calculate the SO interaction functions \( L_{nn'}(k) \) using Eq. (5), it is more convenient to treat them as parameters of the model, which satisfy certain symmetry-imposed conditions. Since the Hamiltonian (4) is Hermitian, we have

\[
L_{nn'}(k) = L^{*}_{n'n}(k).
\]
As for the point group operations, it is sufficient to consider the transformations under proper rotations and inversion, since any improper operation (e.g. a mirror reflection in a plane) can be represented as the product of a proper rotation and the inversion \( I \mathbf{r} = -\mathbf{r} \). Under a rotation \( g = R \) about a direction \( \mathbf{n} \) by an angle \( \theta \), the second-quantization operators transform as follows: \( a_{kns}^\dagger \rightarrow \sum_{s'} a_{Rkns}^\dagger U_{ss'}(R) \), where \( U(R) \equiv D^{(1/2)}(R) \) is the spinor representation of the rotation, see Appendix A. Under inversion \( I \), \( a_{kns}^\dagger \rightarrow a_{-kns}^\dagger \). Using the identity \( U(R)\hat{\sigma}U^\dagger(R) = R^{-1}\hat{\sigma} \), we obtain that \( L_{nn'}(k) \) transform like pseudovectors:

\[
R : \quad L_{nn'}(k) \rightarrow RL_{nn'}(R^{-1}k), \tag{7}
\]

\[
I : \quad L_{nn'}(k) \rightarrow L_{nn'}(-k). \tag{8}
\]

Finally, under time reversal \( K \), \( fa_{kns}^\dagger \rightarrow f^*\sum_{s'}(i\sigma_2)_{ss'}a_{-kns'}^\dagger \) (\( f \) is an arbitrary \( c \)-number constant), therefore

\[
K : \quad L_{nn'}(k) \rightarrow -L_{nn'}^*(-k). \tag{9}
\]

Since the Hamiltonian is invariant under all operations \( g \) from the point group, we obtain:

\[
L_{nn'}(k) = gL_{nn'}(g^{-1}k). \tag{10}
\]

In addition, if the time-reversal invariance is not broken, then

\[
L_{nn'}(k) = -L_{nn'}^*(-k). \tag{11}
\]

In a centrosymmetric crystal, \( L_{nn'}(k) = L_{nn'}(-k) \), therefore it follows from Eq. (11) that

\[
L_{nn'}(k) = -L_{nn'}^*(k). \tag{12}
\]

Using Eq. (6) we obtain that the band-diagonal matrix elements of the SO coupling vanish: \( L_{nn}(k) = 0 \). Therefore one needs to include at least two orbital bands in Eq. (4): \( L_{12}(k) = -L_{21}(k) = i\ell(k) \), where the pseudovector \( \ell \) is real, even in \( k \), and satisfies \( \ell(k) = g\ell(g^{-1}k) \). In contrast, in a noncentrosymmetric crystal the constraint (12) is absent, and the effects of SO coupling can be studied in a minimal model with just one orbital band. Setting \( n = 0 \), we have: \( L_{00}(k) = \gamma(k) \), where the pseudovector \( \gamma \) is real, odd in \( k \), and invariant with respect to the point group operations: \( \gamma(k) = g\gamma(g^{-1}k) \).
B. Pseudospin representation

The simplest description of the SO coupling in a noncentrosymmetric crystal is achieved in a single-band minimal model mentioned in the end of the previous section. A serious drawback of such a model is that it includes only the asymmetric SO coupling and thus completely neglects the SO coupling of electrons with atomic cores. The latter, which is insensitive to the spatial arrangement of the atoms in the crystal, can be important in compounds with heavy atoms. This problem can be remedied if one formulates the theory of the electron-lattice SO coupling using a “pseudospin” representation.

We begin by separating the inversion-symmetric and antisymmetric parts of the lattice potential:

\[ U(r) = U_s(r) + U_a(r), \]

where

\[ U_s(r) = \frac{U(r) + U(-r)}{2}, \quad U_a(r) = \frac{U(r) - U(-r)}{2}. \]

The Hamiltonian (1) can then be represented as follows:

\[ \hat{H} = \hat{H}_s + \hat{H}_a, \]

where

\[ \hat{H}_s = \frac{\hat{p}^2}{2m} + U_s(r) + \hbar \frac{4m^2c^2}{2} \sigma [\nabla U_s(r) \times \hat{p}], \]

\[ \hat{H}_a = U_a(r) + \hbar \frac{4m^2c^2}{2} \sigma [\nabla U_a(r) \times \hat{p}]. \]

Next, we diagonalize the inversion-symmetric part of the Hamiltonian:

\[ \hat{H}_s |k\mu\alpha\rangle = \epsilon_{\mu}(k) |k\mu\alpha\rangle. \]

The spectrum consists of the bands that are two-fold degenerate at each \( k \), because of the combined symmetry operation \( KI \). The index \( \mu \) labels the bands, while \( \alpha = 1, 2 \) distinguishes two orthonormal states within the same band (the “pseudospin states”), which are defined as follows:

\[ |k\mu2\rangle \equiv KI |k\mu1\rangle. \]

Explicitly:

\[ |k\mu\alpha\rangle = \frac{1}{\sqrt{V}} \begin{pmatrix} u_{k\mu\alpha}(r) \\ v_{k\mu\alpha}(r) \end{pmatrix} e^{ikr}, \quad u_{k\mu2}(r) = v_{k\mu1}^*(-r), \quad v_{k\mu2}(r) = -u_{k\mu1}^*(-r). \]

Here \( u_{k\mu\alpha}(r) \) and \( v_{k\mu\alpha}(r) \) have the same periodicity as the crystal lattice. There is still freedom in the relative “orientation” of the eigenspinors at different points in the Brillouin zone. Following Ref. 43, we choose the pseudospin states at each \( k \) in such a way that they transform under the point group operations (including inversion) and time reversal in the same manner as the pure spin eigenstates, see Eq. (A3). Starting from some wave vector...
in the fundamental domain of the first Brillouin zone, one can use the expressions

\[ g | \mathbf{k}_0 \mu \alpha \rangle = \sum_{\beta} | g \mathbf{k}_0, \mu \beta \rangle D_{\beta \alpha}^{(1/2)}(g), \quad (16) \]

\[ K | \mathbf{k}_0 \mu \alpha \rangle = \sum_{\beta} (i \sigma_2)_{\alpha \beta} | - \mathbf{k}_0, \mu \beta \rangle, \quad (17) \]

to define the pseudospin states at all other wave vectors belonging to the star of \( \mathbf{k}_0 \).

We can now calculate the matrix elements of the antisymmetric part of the Hamiltonian in the pseudospin basis (15):

\[ \langle \mathbf{k} \mu \alpha | \hat{H}_a | \mathbf{k}' \nu \beta \rangle = \delta_{k, k'} X_{\alpha \beta}^{\mu \nu}(k), \quad \text{where} \quad X_{\alpha \beta}^{\mu \nu}(k) = -X_{\alpha \beta}^{\nu \mu}(-k) \quad \text{due to the odd parity of} \quad \hat{H}_a. \]

These matrix elements can be expressed, quite generally, in terms of the Pauli matrices in the pseudospin space as follows:

\[ X_{\alpha \beta}^{\mu \nu}(k) = i A_{\mu \nu}(k) \delta_{\alpha \beta} + B_{\mu \nu}(k) \sigma_{\alpha \beta}. \]

[Note that it would be wrong to associate the first and the second terms in this expression with the potential and the SO contributions in Eq. (14), respectively. For instance, \( \langle \mathbf{k} \mu \alpha | U_a | \mathbf{k}' \nu \beta \rangle \) is not proportional to \( \delta_{\alpha \beta} \), in general.] The Hamiltonian of the system in the pseudospin representation has the following form:

\[ H = \sum_{\mathbf{k}, \mu \nu} \sum_{\alpha \beta = 1, 2} [\epsilon_{\mu}(k) \delta_{\mu \nu} \delta_{\alpha \beta} + i A_{\mu \nu}(k) \delta_{\alpha \beta} + B_{\mu \nu}(k) \sigma_{\alpha \beta}] b_{k \mu \alpha}^\dagger b_{k \nu \beta}. \quad (18) \]

Here, in contrast to Eq. (14), the effects of the inversion-antisymmetric part of the lattice potential (the last two terms) are explicitly separated from the inversion-symmetric part (the first term), the latter containing all the information about the intra-atomic SO coupling.

The parameters of the Hamiltonian (18) must satisfy a set of rather restrictive conditions, which are imposed by the symmetry of the system. Taking into account the requirements of Hermiticity and time-reversal invariance, see Sec. II A, we obtain that \( A_{\mu \nu}(k) \) and \( B_{\mu \nu}(k) \) are real, odd in \( k \), and satisfy \( A_{\mu \nu}(k) = -A_{\nu \mu}(k) \) and \( B_{\mu \nu}(k) = B_{\nu \mu}(k) \). As for the point group invariance, proper and improper operations have to be considered separately, using the fact that, by construction, the pseudospin states transform in the same way as the pure spinor states considered in Sec. II A. For a proper rotation \( R \) we have: \( A_{\mu \nu}(k) = A_{\mu \nu}(R^{-1}k) \) and \( B_{\mu \nu}(k) = R B_{\mu \nu}(R^{-1}k) \). For an improper operation which is a product of a rotation \( \tilde{R} \) and inversion \( I \) we have: \( A_{\mu \nu}(k) = -A_{\mu \nu}(\tilde{R}^{-1}k) \) and \( B_{\mu \nu}(k) = -\tilde{R} B_{\mu \nu}(\tilde{R}^{-1}k) \).

The antisymmetric SO coupling can, in general, lift the pseudospin degeneracy of the bands \( \epsilon_{\mu}(k) \). Since the second term in Eq. (18) is invariant under arbitrary rotations in the pseudospin space, the degeneracy is removed only if \( B_{\mu \nu}(k) \neq 0 \). The bands always remain at least two-fold degenerate at the center of the Brillouin zone, because \( B_{\mu \nu}(0) = 0 \).
C. One-band Hamiltonian

The electron band structure in noncentrosymmetric crystals has some peculiar features, e.g., a nontrivial topology of the band wavefunctions, which have a significant effect on the dynamics of quasiparticles. We shall study those features using a model in which just one band is kept. This can be justified if the energy splitting of the two pseudospin states with the same band index $\mu$ due to the antisymmetric SO coupling is much smaller than the separation between the bands with different $\mu$. In the one-band model, setting $\mu = \nu = 0$ we have $A_{00}(k) = 0$ and $B_{00}(k) \equiv \gamma(k)$, so that the Hamiltonian (18) is reduced to the following form:

$$H = \sum_k \sum_{\alpha,\beta = 1,2} [\epsilon_0(k)\delta_{\alpha\beta} + \gamma(k)\sigma_{\alpha\beta}]b_{k\alpha}^\dagger b_{k\beta}$$

(19)

Here the band dispersion satisfies $\epsilon_0(k) = \epsilon_0(-k)$ and $\epsilon_0(k) = \epsilon_0(g^{-1}k)$. The antisymmetric electron-lattice SO coupling is described by a real pseudovector function $\gamma(k)$, which is odd in $k$. According to Sec. [13] it has the following symmetry properties with respect to the point group operations: Under a proper rotation $R$, $\gamma(k) = R\gamma(R^{-1}k)$, while under an improper operation $I\tilde{R}$, $\gamma(k) = -\tilde{R}\gamma(\tilde{R}^{-1}k)$. Lowest-order polynomial expressions for $\gamma(k)$ for all 21 noncentrosymmetric point groups are given in Table [14]. The SO coupling Hamiltonian of the form (19) is sometimes called the generalized Rashba model, after Ref. [44], in which the particular case with $\gamma(k) = a(k_y\hat{x} - k_x\hat{y})$ was considered. The original Rashba model has been extensively used (see, e.g., Ref. [45]) to describe the properties of quasi-two-dimensional semiconductors which are noncentrosymmetric due to the asymmetry of the confining potential.

When it is necessary to take into account the crystal periodicity, the basis functions should be represented as the lattice Fourier series: $\gamma(k) = \sum_n \gamma_n \sin kR_n$, where summation goes over the sites $R_n$ of the Bravais lattice which cannot be transformed one into another by inversion. For example, in the case of a simple tetragonal lattice, which is realized in CePt$_3$Si (point group $G = C_{4v}$, space group $P4mm$), we have in the nearest-neighbor approximation:

$$\gamma(k) = a(\hat{x}\sin k_yd - \hat{y}\sin k_xd),$$

(20)

where $d$ is the lattice spacing in the basal plane. In order to obtain a nonzero $z$-component of the SO coupling, one has to go beyond the nearest-neighbor approximation.
TABLE I: Representative expressions for the antisymmetric SO coupling for all noncentrosymmetric point groups (using both Schoenflies and International notations); $a_i$ and $a$ are real constants, $b_i$ and $b$ are complex constants, and $k_{\pm} = k_x \pm i k_y$. In the right column, the types of the symmetry-imposed zeros of the SO coupling are listed.

| $G$   | $\gamma(k)$                                                                 | zeros of $\gamma(k)$ |
|-------|----------------------------------------------------------------------------|-----------------------|
| $C_1$ (1) | $(a_1 k_x + a_2 k_y + a_3 k_z) \hat{x} + (a_4 k_x + a_5 k_y + a_6 k_z) \hat{y} + (a_7 k_x + a_8 k_y + a_9 k_z) \hat{z}$ | point                 |
| $C_2$ (2) | $\gamma(k) = a_1 k_x \hat{x} + a_2 k_y \hat{y} + a_3 k_z \hat{z}$ | point                 |
| $C_s$ (m) | $\gamma(k) = a_1 k_z \hat{x} + a_2 k_z \hat{y} + (a_3 k_x + a_4 k_y) \hat{z}$ | point                 |
| $D_2$ (222) | $\gamma(k) = a_1 k_x \hat{x} + a_2 k_y \hat{y} + a_3 k_z \hat{z}$ | point                 |
| $C_{2v}$ (mm2) | $\gamma(k) = a_1 k_y \hat{x} + a_2 k_x \hat{y} + i a_3 (k_{+}^2 - k_{-}^2) k_z \hat{z}$ | line                  |
| $C_4$ (4) | $\gamma(k) = a_1 k_x \hat{x} + a_2 k_y \hat{y} + a_3 k_z \hat{z}$ | point                 |
| $S_4$ (4) | $\gamma(k) = a_1 k_x \hat{x} + a_2 k_y \hat{y} + (a_3 k_x - a_4 k_y) \hat{z}$ | line                  |
| $D_4$ (422) | $\gamma(k) = a_1 (k_x \hat{x} + k_y \hat{y}) + a_2 k_z \hat{z}$ | point                 |
| $C_{4v}$ (4mm) | $\gamma(k) = a_1 (k_y \hat{x} - k_x \hat{y}) + a_2 (k_{+}^4 - k_{-}^4) k_z \hat{z}$ | line                  |
| $D_{2d}$ (42m) | $\gamma(k) = a_1 (k_x \hat{x} - k_y \hat{y}) + a_2 (k_{+}^2 + k_{-}^2) k_z \hat{z}$ | line                  |
| $C_3$ (3) | $\gamma(k) = a_1 k_x \hat{x} + a_2 k_y \hat{y} + a_3 k_z \hat{z}$ | point                 |
| $D_3$ (32) | $\gamma(k) = a_1 (k_x \hat{x} + k_y \hat{y}) + a_2 k_z \hat{z}$ | point                 |
| $C_{3v}$ (3m) | $\gamma(k) = a_1 (k_y \hat{x} - k_z \hat{y}) + a_2 (k_{+}^3 + k_{-}^3) \hat{z}$ | line                  |
| $C_6$ (6) | $\gamma(k) = a_1 k_x \hat{x} + a_2 k_y \hat{y} + a_3 k_z \hat{z}$ | point                 |
| $C_{3h}$ (6) | $\gamma(k) = b_1 k_{+}^2 + b_{-}^2 k_{-}^2) k_z \hat{x} + i (b_1 k_{+}^2 - b_{-}^2 k_{-}^2) k_z \hat{y} + (b_2 k_{+}^2 + b_{-}^2 k_{-}^2) \hat{z}$ | line                  |
| $D_6$ (622) | $\gamma(k) = a_1 (k_x \hat{x} + k_y \hat{y}) + a_2 k_z \hat{z}$ | point                 |
| $C_{6v}$ (6mm) | $\gamma(k) = a_1 (k_y \hat{x} - k_z \hat{y}) + a_2 (k_{+}^6 - k_{-}^6) k_z \hat{z}$ | line                  |
| $D_{3h}$ (6m2) | $\gamma(k) = a_1 [i (k_{+}^2 - k_{-}^2) k_z \hat{x} - (k_{+}^2 + k_{-}^2) k_z \hat{y}] + a_2 (k_{+}^3 - k_{-}^3) \hat{z}$ | line                  |
| $T$ (23) | $\gamma(k) = a(k_x \hat{x} + k_y \hat{y} + k_z \hat{z})$ | point                 |
| $O$ (432) | $\gamma(k) = a(k_x \hat{x} + b_1 k_y \hat{y} + k_z \hat{z})$ | point                 |
| $T_d$ (43m) | $\gamma(k) = a[k_x (k_{+}^2 - k_{-}^2) \hat{x} + k_y (k_{+}^2 - k_{-}^2) \hat{y} + k_z (k_{+}^2 - k_{-}^2) \hat{z}]$ | 3 lines               |

The Hamiltonian can be diagonalized by a unitary transformation $b_k = \sum_\lambda u_{\alpha \lambda}(k)c_{k\lambda}$, where $\lambda = \pm$, and

$$u_{1\lambda} = \frac{1}{\sqrt{2}} \sqrt{1 + \frac{\gamma_z}{|\gamma|}}, \quad u_{2\lambda} = \frac{\lambda}{\sqrt{2}} \sqrt{\frac{\gamma_x + i \gamma_y}{\gamma_x \gamma_y + \gamma_y^2}} \sqrt{1 - \frac{\gamma_z}{|\gamma|}},$$

(21)
with the following result:

$$H = \sum_{k} \sum_{\lambda=\pm} \xi_{\lambda}(k) c_{k \lambda}^{\dagger} c_{k \lambda}. \quad (22)$$

The energy of the fermionic quasiparticles in the $\lambda$th band is given by

$$\xi_{\lambda}(k) = \epsilon_0(k) + \lambda |\gamma(k)|, \quad (23)$$

The bands are even in $k$ despite the antisymmetry of the SO coupling, which is a manifestation of the Kramers degeneracy: The states $|k \lambda\rangle$ and $|-k, \lambda\rangle$ are related by time reversal and therefore have the same energy. In contrast, the pseudospin degeneracy of the electron states at the same $k$ is lifted by the SO coupling $\gamma(k)$, which can be viewed as an effective “Zeeman magnetic field” acting on the electron spins. For an excitation with a given wave vector $k$, the spin direction is either parallel $(\lambda = +)$ or antiparallel $(\lambda = -)$ to $\gamma(k)$. In the particular case of $\gamma(k) \propto k$, the band index $\lambda$ has the meaning of the helicity, which is the spin projection on the direction of momentum. For brevity, we will be referring to the bands (23) as the helicity bands for arbitrary $\gamma(k)$. In real noncentrosymmetric metals, the SO splitting between the helicity bands is strongly anisotropic. Its magnitude can be characterized by $E_{SO} = 2 \max_k |\gamma(k)|$. For instance, in CePt$_3$Si $E_{SO}$ ranges from 50 to 200 meV (Ref. 46), while in Li$_2$(Pd$_{1-x}$Pt$_x$)$_3$B $E_{SO}$ is 30 meV in Li$_2$Pd$_3$B, reaching 200 meV in Li$_2$Pt$_3$B (Ref. 47).

One can also consider a more general case of a magnetic noncentrosymmetric crystal, e.g., MnSi (Ref. 48). Neglecting the spatial variation of the magnetization due to domain walls or a helical modulation, the exchange field can be represented in the simplest case by a constant pseudovector $h$. Its effect on the electronic structure can be described by the Hamiltonian (19), if one replaces $\gamma(k)$ by the generalized “Zeeman field” $\gamma(k) + h$. In this case, the time-reversal symmetry is broken, and the helicity bands are no longer even in $k$:

$$\xi_{\lambda}(k) = \epsilon_0(k) + \lambda |\gamma(k) + h| \neq \xi_{\lambda}(-k) = \epsilon_0(k) + \lambda |\gamma(k) - h|. \quad (24)$$

D. Band degeneracies

According to Table II, the helicity bands are degenerate at some points in the Brillouin zone, where the antisymmetric SO coupling vanishes. In particular, this happens at $k = 0$, which is a trivial consequence of the fact that $\gamma(k)$ is odd in $k$. For some point groups, the bands are degenerate along whole lines: For the uniaxial groups $C_{2v}$, $S_4$, $C_{4v}$, $C_{3v}$, $C_{3h}$, and
$C_{6v}$, as well as for the dihedral groups $D_{2d}$ and $D_{3h}$, the SO band splitting vanishes along the principal axis $k_x = k_y = 0$, while for the full tetrahedral group $T_d$, it vanishes along the three mutually perpendicular axes $k_x = k_y = 0$, $k_y = k_z = 0$, and $k_z = k_x = 0$. Taking into account the periodicity of the reciprocal space, one gets additional band degeneracies. For example, the SO coupling in a simple tetragonal lattice vanishes along the following lines in the first Brillouin zone: $k_x = 0, \pm \pi/a, k_y = 0, \pm \pi/a$, see Eq. (20). It will be shown in Sec. III B that the band degeneracies can be viewed as “topological defects” in $k$-space, which create a nontrivial topological structure of the band electron wavefunctions.

It is important to note that the expressions from Table I are actually applicable to all components of the antisymmetric SO coupling $B_{\mu\nu}(k)$, see Sec. III B. Therefore, a symmetry-imposed zero of $\gamma(k)$ will not be removed even if the interband elements of the antisymmetric SO coupling are taken into account. This implies that, while the bands are nondegenerate almost everywhere in the Brillouin zone, each of the bands will always touch at least one of the other bands at a high-symmetry point or along a high-symmetry line. This is markedly different from the centrosymmetric case, where the band degeneracies are possible in some cases,[49] but they are not mandatory.

In addition to the zeros imposed by symmetry, the antisymmetric SO coupling might vanish at some $k$ for accidental reasons. It is easy to show that, while the isolated point zeros cannot be removed by a small variation in the parameters of the system (i.e. are topologically stable), the accidental lines of zeros can be removed and therefore are exceedingly improbable. The proof is based on the observation that the SO coupling interaction $\gamma(k)$ away from the degeneracies defines a mapping, $k \rightarrow \hat{\gamma}(k)$, of $k$-space onto a sphere $S^2$, where $\hat{\gamma} = \gamma/|\gamma|$. Since the second homotopy group of the sphere is nontrivial: $\pi_2(S^2) = \mathbb{Z}$ (see, e.g., Ref. 50), the accidental point zeros are topologically stable. On the other hand, $\pi_1(S^2) = 0$, and therefore the accidental lines of zeros are not topologically stable. They become stable in a “two-dimensional” limit $\gamma_z(k) \equiv 0$, which might be realized in a strongly-layered crystal, or for an electron gas confined in a plane. In this case, the $\hat{\gamma}(k)$ traces out a circle $S^1$, and the first homotopy group becomes nontrivial: $\pi_1(S^1) = \mathbb{Z}$. Less formally, the stability of the band degeneracy points can also be understood using the following argument. Suppose there is an isolated zero of $\gamma(k)$ at some $k = k_0$. If the parameters of the system are changed so that $\gamma$ is replaced by $\gamma + \delta\gamma$, then one can, in general, neglect the variation of $\delta\gamma$ near $k_0$. Assuming that $\delta\gamma$ is small enough, the new SO coupling still
has an isolated zero, at \( k_0 + \delta k \), where \( \delta k \sim \mathcal{O}(\delta \gamma) \). Applying this argument to a magnetic noncentrosymmetric crystal, see Sec. III C, we see that a sufficiently weak exchange field merely shifts the band degeneracy point away from \( k = 0 \), but does not remove it.

### III. SEMICLASSICAL DYNAMICS OF QUASIPARTICLES

The standard derivation of the semiclassical equations of motion of the fermionic quasiparticles in the \( \lambda \)th band in the presence of external magnetic and/or electric fields is based on the assumption that the dynamics is generated by a classical band Hamiltonian \( \mathcal{H}_\lambda = \xi_\lambda(P/\hbar) - e\phi \), which is obtained from the band dispersion \((23)\). Here \( P = p + (e/c)A \) is the kinetic momentum, \( p \) is the canonical momentum, \( A(r) \) and \( \phi(r) \) are the vector and scalar potentials, respectively, and \( e \) is the absolute value of the electron charge. When the classical trajectory is found, it can be used to “re-quantize” the system by inserting the corresponding action integral into the Bohr-Sommerfeld condition to find the quantum energy levels. It is this approach that has been extensively used, in particular, in the theory of quantum magnetic oscillations in metals. Its drawback is that it represents only the zeroth order term in the semiclassical expansion and therefore does not take into account any of the important quantum corrections. These include, in addition to the Berry phase effects mentioned in the Introduction, also the interaction of the magnetic moment of the band quasiparticles with the external field.

In this section we develop a semiclassical theory of quasiparticle dynamics near the Fermi energy in the model \((19)\), with the lowest-order quantum corrections all taken into account. It is convenient to express the Hamiltonian in terms of the momentum \( p = \hbar k \), instead of the wave vector \( k \), and introduce the following notations for the quasiparticle energy and the SO coupling:

\[
\varepsilon(p) = \varepsilon_F + \varepsilon_0 \left( \frac{p}{\hbar} \right), \quad g(p) = \gamma \left( \frac{p}{\hbar} \right),
\]

or \( g(p) = \gamma(p/\hbar) + \hbar \) in the magnetic case. Note that in this section we do not include the chemical potential in the definition of the quasiparticle energy, e.g., \( \varepsilon(p) = p^2/(2m^*) \) in the effective mass approximation. The external electric and magnetic fields, \( E \) and \( B \), are assumed to vary slowly in comparison to the typical wavelength of the quasiparticles, which is of the order of the inverse Fermi wave vector \( k_F^{-1} \). The effects of the fields are described by a Hamiltonian which can be written as an expansion in powers of \( B \), and
in which the classical canonical momentum $\mathbf{p}$ is replaced by the kinetic momentum operator $\hat{\mathbf{P}} = \hat{\mathbf{p}} + (e/c) \mathbf{A}(\mathbf{r})$ (the Peierls substitution). In our case, this Hamiltonian has the following form:

$$\hat{H}_{\alpha\beta} = \varepsilon(\hat{\mathbf{P}})\delta_{\alpha\beta} + g(\hat{\mathbf{P}})\sigma_{\alpha\beta} - e\phi(\mathbf{r})\delta_{\alpha\beta} + \mu_m \mathbf{B}\sigma_{\alpha\beta}.$$  \hspace{1cm} (24)

The last term represents the interaction of the magnetic moment of the band electrons (which contains both spin and orbital contributions) with the magnetic field. While in general it can be momentum-dependent and have a tensor structure, we neglect such complications here and assume that $\mu_m = (g/2)\mu_B$, where $g$ is the Landé factor and $\mu_B$ is the Bohr magneton. Note that the order of application of the components of the kinetic momentum operator is important, because they do not commute: $[\hat{P}_i, \hat{P}_j] = -i(\hbar e/c)F_{ij}$, where $F_{ij} = \nabla_i A_j - \nabla_j A_i = \sum_k e_{ijk}B_k$ is the magnetic field written as an antisymmetric tensor. Expressions of the form $f(\hat{\mathbf{P}})$ should be understood in the following sense: If one defines the Fourier-transform of the function $f(\mathbf{p})$ as follows: $f(\mathbf{p}) = \int d\mathbf{\rho} \tilde{f}(\mathbf{\rho}) e^{-i(\mathbf{p}\cdot\mathbf{\rho})/\hbar}$, then

$$f(\hat{\mathbf{P}}) = \int d\mathbf{\rho} \tilde{f}(\mathbf{\rho}) e^{-i(\hat{\mathbf{P}}\cdot\mathbf{\rho})/\hbar}.$$ \hspace{1cm} (25)

We shall study the properties of the Hamiltonian \cite{24} in the semiclassical approximation, which is applicable when the action, $S$, calculated along a classical trajectory is much greater than Planck’s constant $\hbar$. For an electron moving in a cyclotron orbit or radius $r_c$, $S \sim p_F r_c \sim \epsilon_F / \omega_c$, where $p_F = \hbar k_F$ is the characteristic Fermi momentum and $\omega_c$ the characteristic cyclotron frequency. The semiclassical parameter is therefore given by

$$\frac{\hbar \omega_c}{\epsilon_F} \ll 1.$$ \hspace{1cm} (26)

Another requirement is that the semiclassical dynamics of the quasiparticles can be studied independently in each of the helicity bands, i.e., in other words, there is no interband transitions. To satisfy this requirement, one has to assume that the spin evolves adiabatically along the classical trajectory in such a way that the helicity is conserved.\cite{45} In the presence of external magnetic field, the direction of the “Zeeman field” $g(\mathbf{p})$ is continuously changing as the excitation is moving along its cyclotron orbit. In order for the spin to be able to follow the direction of $g(\mathbf{p})$ adiabatically, the frequency of the orbital motion, i.e. $\omega_c$, must be much smaller than the frequency associated with the $g(\mathbf{p})$, whose typical value is $E_{SO}/\hbar$ (assuming that the SO band splitting remains nonzero and does not vary considerably along
the orbit, and that the exchange field in the magnetic case is sufficiently small). Thus we have
\[
\frac{\hbar \omega_c}{E_{SO}} \ll 1. \tag{27}
\]
Finally, there are additional constraints on the magnitudes of the applied fields, preventing the electric and magnetic breakdowns due to the interband transitions. According to Ref. 51, the following conditions should hold in order for a single-band semiclassical description to work: \(eEa \ll E_{gap}^2/\epsilon_F\) and \(\hbar \omega_c \ll E_{gap}^2/\epsilon_F\), where the length \(a\) is of the order of the lattice constant and \(E_{gap}\) is the energy splitting between the nearest bands. For the model \(E_{gap} \sim E_{SO}\), and one can write
\[
\frac{\hbar \omega_c}{E_{SO}} \ll \frac{E_{SO}}{\epsilon_F}. \tag{28}
\]
Since typically \(E_{SO} \lesssim \epsilon_F\) in noncentrosymmetric metals, this last condition is in fact stronger than either of the inequalities (26) and (27).

The assumption of the absence of the interband transitions fails for sufficiently strong fields, or in the vicinity of the band degeneracy points on the Fermi surface. We consider only those situations, determined by the field direction and the band structure, in which the semiclassical trajectories of the quasiparticles in the momentum space never come close to the band degeneracies.

### A. Derivation of semiclassical equations of motion

Our derivation of the semiclassical equations of motion follows the general scheme for multicomponent wavefunctions developed in Ref. 42, with some modifications relevant specifically for a noncentrosymmetric crystal in a magnetic field, taking into account the SO coupling and the Zeeman interaction. The idea is to make the Hamiltonian \(24\) a diagonal \(2 \times 2\) operator, whose matrix elements (the “band Hamiltonians”) would then be amenable to the usual semiclassical treatment.

We are looking for a unitary operator \(\hat{U}(\mathbf{r}, \mathbf{p})\), which satisfies \(\hat{U}^\dagger(\mathbf{r}, \mathbf{p})\hat{H}(\mathbf{r}, \mathbf{p})\hat{U}(\mathbf{r}, \mathbf{p}) = \hat{H}(\mathbf{r}, \mathbf{p})\) and \(\hat{U}^\dagger(\mathbf{r}, \mathbf{p})\hat{U}(\mathbf{r}, \mathbf{p}) = \hat{\sigma}_0\), where \(\hat{H} = \text{diag}(\hat{H}_+, \hat{H}_-). The operators \(\hat{U}\) and \(\hat{H}\) can be obtained by applying the Weyl quantization to the corresponding Weyl symbols in a phase space, \(\hat{U}_W(\Gamma)\) and \(\hat{H}_W(\Gamma)\), where \(\Gamma = (\mathbf{r}, \mathbf{p})\) is a shorthand notation for canonical positions and momenta. We recall (see, e.g., Ref. 52 and the references therein) that the
Weyl symbol of an operator $\hat{A} = A(\mathbf{r}, \mathbf{p})$ is defined by the Wigner transformation as follows:

$$A_W(\Gamma) = \int d^3\rho \left< \mathbf{r} + \frac{\mathbf{p}}{2} \right| \hat{A} \left| \mathbf{r} - \frac{\mathbf{p}}{2} \right> e^{-(i/\hbar)\mathbf{pp}}. \tag{29}$$

Given the Weyl symbol, the operator is restored using

$$\left< \mathbf{r} \right| \hat{A} \left| \mathbf{r}' \right> = \int \frac{d^3p}{(2\pi\hbar)^3} A_W \left( \frac{\mathbf{r} + \mathbf{r}'}{2}, \mathbf{p} \right) e^{(i/\hbar)\mathbf{p}(\mathbf{r} - \mathbf{r}')} \tag{30}$$

The Weyl symbol of a product can be conveniently expressed by the Moyal formula:

$$(\hat{A}\hat{B})_W(\Gamma) = \exp \left[ \frac{i\hbar}{2} \left( \frac{\partial}{\partial \mathbf{r}} \frac{\partial}{\partial \mathbf{p}'} - \frac{\partial}{\partial \mathbf{p}} \frac{\partial}{\partial \mathbf{r}'} \right) \right] A_W(\Gamma)B_W(\Gamma') |_{\Gamma'} = A_W(\Gamma)B_W(\Gamma) + \frac{i\hbar}{2} \{A_W(\Gamma), B_W(\Gamma)\} + \mathcal{O}(\hbar^2), \tag{31}$$

where $\{A_W, B_W\}$ is the usual Poisson bracket. In our case, the Weyl symbols $\hat{U}_W(\Gamma)$ and $\hat{H}_W(\Gamma) = \text{diag}[\mathcal{H}_+(\Gamma), \mathcal{H}_-(\Gamma)]$ are $2 \times 2$ matrix functions in the phase space, which are found from the equations

$$(\hat{U}^\dagger\hat{H}\hat{U})_W = \hat{\mathcal{H}}_W, \quad (\hat{U}^\dagger\hat{U})_W = \hat{\sigma}_0. \tag{32}$$

The solutions can be sought in the form of semiclassical expansions: $\hat{U}_W = \hat{U}_0 + \hat{U}_1 + \mathcal{O}(\hbar^2)$ and $\hat{H}_\lambda = \mathcal{H}_{0,\lambda} + \mathcal{H}_{1,\lambda} + \mathcal{O}(\hbar^2)$, where $\hat{U}_1$ and $\mathcal{H}_{1,\lambda}$ are of the order of $\hbar$. We shall focus on the lowest two orders in $\hbar$.

First, let us show that the semiclassical expansion of the Weyl symbol of the Hamiltonian $\hat{H}$ has the following form: $\hat{H}_W = \hat{H}_0 + \hat{H}_1 + \mathcal{O}(\hbar^2)$, where

$$\hat{H}_0(\Gamma) = \varepsilon(\mathbf{P})\hat{\sigma}_0 + g(\mathbf{P})\hat{\sigma} - e\phi(\mathbf{r})\hat{\sigma}_0 \tag{33}$$

is the classical counterpart of Eq. (24), $\mathbf{P} = \mathbf{p} + (e/c)\mathbf{A}(\mathbf{r})$, and

$$\hat{H}_1(\Gamma) = \mu_m \mathbf{B}(\mathbf{r})\hat{\sigma} \tag{34}$$

(we consider the general case, in which both the magnetic and electric fields can be nonuniform). It is easy to see that there is no linear in $\hbar$ contributions from the first three terms in Eq. (24). One has to prove this statement only for the first and second terms, which depend on $\hat{\mathbf{P}}$. Let us consider an operator $\hat{f} = f(\mathbf{P})$. Expanding the exponential in Eq. (25), we obtain for its Weyl symbol:

$$f_W = \sum_{n=0}^{\infty} \sum_{i_1, \ldots, i_n} A_{i_1 \ldots i_n} (\hat{P}_{i_1} \hat{P}_{i_2} \ldots \hat{P}_{i_n})_W, \tag{35}$$
where $A_{i_1...i_n} = (1/n!){\partial^n f(p)}/{\partial p_{i_1}...\partial p_{i_n}}|_{p=0}$ is completely symmetric with respect to the permutations of $i_1, i_2, ... i_n$. The Weyl symbols of the operator products on the right-hand side can be obtained by applying the Moyal formula and using the fact that $(\hat{P})_W = P$:

$$
(\hat{P}_{i_1}\hat{P}_{i_2}...\hat{P}_{i_n})_W = P_{i_1}(\hat{P}_{i_2}\hat{P}_{i_3}...\hat{P}_{i_n})_W + \frac{i\hbar}{2}\{P_{i_1}, (\hat{P}_{i_2}\hat{P}_{i_3}...\hat{P}_{i_n})_W\} + \mathcal{O}(\hbar^2)
$$

$$
= P_{i_1}(\hat{P}_{i_2}\hat{P}_{i_3}...\hat{P}_{i_n})_W + \frac{i\hbar}{2}\{P_{i_1}, P_{i_2}P_{i_3}...P_{i_n}\} + \mathcal{O}(\hbar^2)
$$

$$
= P_{i_1}(\hat{P}_{i_2}\hat{P}_{i_3}...\hat{P}_{i_n})_W + \frac{i\hbar}{2}\{\{P_{i_1}, P_{i_2}\}\hat{P}_{i_3}...\hat{P}_{i_n} + P_{i_2}\{P_{i_1}, P_{i_3}\}\hat{P}_{i_4}...\hat{P}_{i_n} + ...\} + \mathcal{O}(\hbar^2).
$$

The last line follows from the chain-rule property of the Poisson bracket: $\{a, bc\} = \{a, b\}c + b\{a, c\}$. Since $\{P_{i_1}, P_{i_2}\} = -\{P_{i_2}, P_{i_1}\}$, etc, each term in the square brackets vanishes when multiplied by the symmetric coefficients $A_{i_1...i_n}$ and summed over $i_1, ..., i_n$. Repeating this argument for the Weyl symbols of the remaining operator products, we find:

$$
(\hat{P}_{i_1}\hat{P}_{i_2}...\hat{P}_{i_n})_W = P_{i_1}P_{i_2}...P_{i_n} + \mathcal{O}(\hbar^2).\quad \text{Substitution into Eq. (35) gives } f_W = f(P) + \mathcal{O}(\hbar^2).
$$

Applying this result to the matrix elements of first two terms in the Hamiltonian, we arrive at Eq. (33). The only linear in $\hbar$ correction to the Weyl symbol of the Hamiltonian comes from the magnetic moment interaction, because $\mu_m \sim \mu_B$ is proportional to Planck’s constant.

In this context, one might wonder about the legitimacy of including the SO coupling term in the classical Weyl symbol $\hat{H}_0$, since formally it is also proportional to $\hbar$, which can be traced back to the general expression for the SO interaction in Eq. (11). We recall that the actual semiclassical expansion parameter is not Planck’s constant itself, but the dimensionless ratio $\hbar\omega_c/\epsilon_F$, see Eq. (20). While the magnetic moment interaction is indeed smaller than the quasiparticle energy $\epsilon(p)$ by a factor of $\mu_mB/\epsilon_F \sim \hbar\omega_c/\epsilon_F \ll 1$, the SO coupling does not contain this ratio at all. In fact, the latter is much greater than the former: $E_{SO}/\mu_mB \sim E_{SO}/\hbar\omega_c \gg 1$, see Eq. (27), which justifies its treatment as a part of $\hat{H}_0$.

Using the Moyal formula, one can solve Eqs. (32) and obtain the Weyl symbols of the band Hamiltonian operators: $\mathcal{H}_\lambda = \mathcal{H}_{0,\lambda} + \mathcal{H}_{1,\lambda} + \mathcal{O}(\hbar^2)$, where $\lambda = \pm$. The leading terms in the semiclassical expansions,

$$
\mathcal{H}_{0,\lambda}(\Gamma) = \epsilon(P) + \lambda|g(P)| - e\phi(r),
$$

are just the eigenvalues of $\hat{H}_0$, see Eq. (33). The corresponding eigenvectors are given by
the following expressions:

$$
\tau_{\lambda,1}(P) = \frac{1}{\sqrt{2}} \sqrt{1 + \lambda \frac{g_z}{g}}, \quad \tau_{\lambda,2}(P) = \frac{\lambda}{\sqrt{2}} \frac{g_z + ig_y}{\sqrt{g_x^2 + g_y^2}} \sqrt{1 - \lambda \frac{g_z}{g}},
$$

(37)

cf. Eq. (21). The first quantum correction can be represented as follows: $H_{1,\lambda} = H_{1,\lambda}^{(1)} + H_{1,\lambda}^{(2)} + H_{1,\lambda}^{(3)}$, where

$$
H_{1,\lambda}^{(1)}(\Gamma) = \sum_{\alpha\beta} \tau_{\lambda,\alpha}^* H_{1,\alpha\beta}^\lambda \tau_{\lambda,\beta},
$$

$$
H_{1,\lambda}^{(2)}(\Gamma) = -\frac{i\hbar}{2} \sum_{\alpha\beta} (H_{0,\alpha\beta} - H_{0,\lambda} \delta_{\alpha\beta}) \{ \tau_{\lambda,\alpha}^*, \tau_{\lambda,\beta} \},
$$

$$
H_{1,\lambda}^{(3)}(\Gamma) = -i\hbar \tau_{\lambda}^* \{ \tau_{\lambda}, H_{0,\lambda} \}.
$$

(38)

These expressions can be derived using a straightforward generalization of the procedure described in Ref. 42.

The quantum band Hamiltonians $\hat{H}_\lambda$ can be derived from $H_{\lambda}(r, p)$ by means of the Weyl quantization, and the wavefunctions of the quasiparticles can be analyzed independently in the two bands. We recall that in the semiclassical approximation, one can seek the (time-independent) wavefunctions in the form $\psi(r) \sim e^{iS(r)/\hbar}$, where the action $S$ satisfies the Hamilton-Jacobi equation $H_{\lambda}(r, \nabla S) = 0$ (Ref. 53). If the system is integrable, then a complete integral of the Hamilton-Jacobi equation can be found, the classical orbits lie on tori in phase space, and the motion along the orbits is quasiperiodic. In this case the quantum energy levels can be obtained by imposing the Bohr-Sommerfeld quantization condition on the action integrals calculated along independent basic contours, $C_i$, on the torus: $\oint_{C_i} p \, dr = 2\pi\hbar (n_i + \gamma_i)$, where $n_i$ is a large integer, and $\gamma_i$ is either 0 or 1/2 (for electrons in metals, the latter possibility is realized, see Ref. 38). When implementing this procedure for our system, we encounter the problem that the classical band Hamiltonians $H_\lambda$ and the associated Hamilton-Jacobi equations are not invariant under the $U(1)$ phase rotations of the eigenvectors, $\tau_\lambda(\Gamma) \to e^{i\theta_\lambda(\Gamma)} \tau_\lambda(\Gamma)$, where $\theta_\lambda$ are arbitrary smooth functions of the phase space coordinates. Indeed, under such transformations, $H_{0,\lambda}$, $H_{1,\lambda}^{(1)}$, and $H_{1,\lambda}^{(2)}$ all remain the same, but $H_{1,\lambda}^{(3)}$ changes, since $-i\tau_\lambda^* \{ \tau_\lambda, H_{0,\lambda} \} \to -i\tau_\lambda^* \{ \tau_\lambda, H_{0,\lambda} \} + \{ \theta_\lambda, H_{0,\lambda} \}$. Furthermore, the classical band Hamiltonians are not invariant under a usual gauge transformation of the vector potential, $A(r) \to A(r) + \nabla f$.

In order to develop a manifestly gauge-independent description of the classical motion, we introduce, following Ref. 42, new coordinates in the phase space for each of the helicity
bands: $\Gamma' = (\mathbf{r}', \mathbf{p}')$, where $r'_i = r_i - i\hbar \tau^*_\lambda \{\tau_\lambda, r_i\}$ and $p'_i = p_i - i\hbar \tau^*_\lambda \{\tau_\lambda, p_i\}$. It is straightforward to show that, in the first order in $\hbar$, the Weyl symbols in the new coordinates take the following form: $H_{\lambda,0}(\Gamma') = H_{\lambda,0}(\Gamma') + H_{\lambda,1}(1)(\Gamma') + H_{\lambda,2}(2)(\Gamma')$, which no longer depends on the phase convention for the eigenvectors $\tau_\lambda$. The action integral along a closed path in phase space can also be expressed in terms of the new coordinates:

$$J = \oint p \, d\mathbf{r} = \oint p' \, d\mathbf{r}' + i\hbar \oint \tau^*_\lambda \, d\tau_\lambda,$$

neglecting the terms of the order of $\hbar^2$. The last term is associated with the Berry phase picked up by the wave function in the course of the semiclassical evolution along the closed path in the parameter space. [32]

The price one pays for the restoration of the gauge invariance is that the new coordinates are noncanonical. In particular, the new positions have nontrivial Poisson brackets:

$$\{r'_i, r'_j\} = i\hbar \left( \frac{\partial \tau^*_\lambda}{\partial p'_i} \frac{\partial \tau_\lambda}{\partial p'_j} - \frac{\partial \tau^*_\lambda}{\partial p'_j} \frac{\partial \tau_\lambda}{\partial p'_i} \right).$$

This expression can be represented in a more compact form using the fact that the eigenvectors (57) depend only on the transformed kinetic momentum $\mathbf{P}' = \mathbf{p}' + (e/c) \mathbf{A}(\mathbf{r}')$. We introduce the Berry connection (or the “vector potential”) in the momentum space:

$$A_{\lambda,i}(\mathbf{P}) = i\tau^*_\lambda(\mathbf{P}) \frac{\partial}{\partial P_i} \tau_\lambda(\mathbf{P}),$$

and also the corresponding curvature tensor:

$$F_{\lambda,ij}(\mathbf{P}) = \frac{\partial A_{\lambda,j}}{\partial P_i} - \frac{\partial A_{\lambda,i}}{\partial P_j} = i \left( \frac{\partial \tau^*_\lambda}{\partial P_i} \frac{\partial \tau_\lambda}{\partial P_j} - \frac{\partial \tau^*_\lambda}{\partial P_j} \frac{\partial \tau_\lambda}{\partial P_i} \right),$$

which can be expressed in terms of the Berry “magnetic field” $\mathbf{B}_\lambda(\mathbf{P}) = \nabla_\mathbf{P} \times \mathbf{A}_\lambda(\mathbf{P})$ as follows: $F_{\lambda,ij} = \sum_k e_{ijk} \mathbf{B}_{\lambda,k}$. Under the phase rotation of the eigenvectors mentioned above, the Berry connection changes: $\mathbf{A}_\lambda \to \mathbf{A}_\lambda + \nabla_\mathbf{P} \theta_\lambda$, while the Berry curvature remains invariant. We shall see in Sec. III B that the Berry field is sensitive to the topology of the band eigenstates. For the Poisson bracket (40) we obtain: $\{r'_i, r'_j\} = \hbar F_{\lambda,ij}(\mathbf{P}')$. Other Poisson brackets, $\{r'_i, p'_j\}$ and $\{p'_i, p'_j\}$, can also be expressed in terms of the Berry curvature, but they still contain the vector potential $\mathbf{A}(\mathbf{r})$ and therefore are not gauge-invariant. To fix this, we make a second change of coordinates, to $\Gamma'' = (\mathbf{r}'', \mathbf{P}'')$, which makes both the Poisson brackets and the Hamiltonian gauge-invariant and independent of the phase choice for the $\tau_\lambda$s.
Dropping the primes, we finally arrive at the following picture. The classical motion of the quasiparticles in the $\lambda$th band is described by the phase space coordinates $\Gamma = (r, P)$, which have the following Poisson brackets:

$$\{r_i, r_j\} = \hbar F_{\lambda, ij},$$

$$\{r_i, P_j\} = \delta_{ij} + \frac{\hbar e}{c} \sum_k F_{\lambda, ik} F_{kj},$$

$$\{P_i, P_j\} = -\frac{e}{c} F_{ij} - \hbar \left( \frac{e}{c} \right)^2 \sum_{kl} F_{ik} F_{\lambda, kl} F_{lj},$$

which are manifestly noncanonical. While the noncanonical structure of the first term in $\{P_i, P_j\}$ is not really surprising and has a purely classical origin, the terms containing the Berry curvature are essentially nonclassical. These terms appeared in our derivation as the linear in $\hbar$ corrections in the semiclassical expansion. The origin of the Berry curvature terms can also be understood using a different argument, which is based on the observation that $r$ and $P$ refer to a particular helicity band and therefore are not the usual positions and momenta. Instead, they are the classical counterparts of the band-projected position and momentum operators, whose commutators in the classical limit reproduce the noncanonical Poisson brackets (43), see Appendix B. We would like also to mention Ref. 54, where it was shown how a nonzero Berry curvature appears in the adiabatic limit (i.e. when the interband transitions are neglected), by imposing the requirement of extended gauge invariance in the phase space on the wave packet dynamics.

We find it convenient to express both the Berry connection and the Berry field using the spherical angle parametrization of the SO coupling $g(P)$:

$$g_x = |g| \sin \alpha \cos \beta, \quad g_y = |g| \sin \alpha \sin \beta, \quad g_z = |g| \cos \alpha.\) The eigenvectors (37) then become

$$\tau_+ (P) = \begin{pmatrix} \cos \frac{\alpha}{2} \\ e^{i\beta} \sin \frac{\alpha}{2} \end{pmatrix}, \quad \tau_- (P) = \begin{pmatrix} \sin \frac{\alpha}{2} \\ -e^{i\beta} \cos \frac{\alpha}{2} \end{pmatrix}.\) (44)

Inserting these expressions in Eq. (41), we obtain:

$$\mathcal{A}_\lambda (P) = -\frac{1}{2} (1 - \lambda \cos \alpha) \frac{\partial \beta}{\partial P},$$

and

$$\mathcal{B}_\lambda (P) = -\frac{\lambda}{2} \sin \alpha \left( \frac{\partial \alpha}{\partial P} \times \frac{\partial \beta}{\partial P} \right).$$

These expressions are valid away from the band degeneracies, where $\alpha$ and $\beta$ are not defined (and where the semiclassical description fails anyway). In the nonmagnetic case, when the
exchange field $h$ is absent, we have $g(-P) = -g(P)$. Therefore, the inversion $P \rightarrow -P$
corresponds to $\alpha \rightarrow \pi - \alpha$ and $\beta \rightarrow \pi + \beta$, which means that $B_\lambda(-P) = -B_\lambda(P)$. In
contrast, if $h \neq 0$, then neither $g(P)$ nor the Berry field have a definite parity under
inversion.

The gauge-invariant classical band Hamiltonians are given, in the first order in $\hbar$, by
$H_\lambda = H_{0,\lambda} + H_{1,\lambda}^{(1)} + H_{1,\lambda}^{(2)}$. Substituting here Eq. (36) and using the last of the Poisson
brackets (43) in Eq. (38), we obtain:

$$H_\lambda(r, P) = \varepsilon(P) + \lambda|g(P)| - e\phi(r) - \hbar m_\lambda(P)B,$$

(47)

where

$$m_\lambda = \frac{-\mu m}{\hbar} \sum_{\alpha\beta} \tau_{\lambda,\alpha}^* \sigma_{\alpha\beta} \tau_{\lambda,\beta} - \frac{i}{2c} \sum_{\alpha\beta} \left( g_{\alpha\beta} \delta_{\alpha\beta} - \lambda|g| \delta_{\alpha\beta} \right) \left( \frac{\partial \tau_{\lambda,\alpha}^*}{\partial P} \times \frac{\partial \tau_{\lambda,\beta}}{\partial P} \right).$$

(48)

can be interpreted as the magnetic moment of the band quasiparticles (divided by $\hbar$). Using
the eigenvectors (37), the first term in Eq. (48) can be written as $m_\lambda^{(1)} = -\lambda(\mu m/\hbar)\hat{g}$, where $\hat{g} = g/|g|$. The second term, which is sometimes called the Rammal-Wilkinson
contribution, takes in our case a relatively simple form. Using the spherical angle
representation (44), we obtain after some straightforward algebra:

$$m_\lambda^{(2)} = -\frac{e}{2c} |g| \sin \alpha \left( \frac{\partial \alpha}{\partial r} \times \frac{\partial \beta}{\partial r} \right).$$

Comparing this with Eq. (46), one finally arrives at the following expression:

$$m_\lambda(P) = -\lambda \frac{\mu m}{\hbar} \hat{g}(P) + \lambda \frac{e}{c} |g(P)| B_\lambda(P).$$

(49)

The first term is consistent with the expression for the intraband magnetic moment discussed,
e.g., in Refs. 19, 20 (the negative sign appears here because the electron charge is equal to
$-e$). The second term [which is smaller than the first one by a factor $(he/\mu m c)(E_{SO}/p_F^2) \sim
E_{SO}/\epsilon_F$], is entirely determined by the Berry field and therefore is sensitive to the topology
of the band eigenstates. Note that, because of the SO coupling, it would be wrong to
associate the first and the second terms in Eq. (49) with, respectively, the spin and the
orbital magnetic moments.

Now we have all necessary ingredients to derive the equations of motion for $r(t)$ and
$P(t)$. The classical dynamics of the band quasiparticles is generated by the Hamiltonians
(47) in the usual fashion: $\dot{\Gamma} = \{\Gamma, H_\lambda(\Gamma)\}$. Using the Poisson brackets (43), we obtain:

$$\frac{dr}{dt} = v_\lambda(P) - \hbar \frac{dP}{dt} \times B_\lambda(P), \quad \frac{dP}{dt} = -eE(r) - \frac{e}{c} \frac{dr}{dt} \times B(r).$$

(50)
where $v_\lambda = \partial H_\lambda / \partial P$. While the second of these equations has a standard Newtonian form, with the Lorentz force on the right-hand side, the first one contains a nonclassical term proportional to the Berry field, which is called the “anomalous velocity”. The importance of the anomalous term was recognized in the early theories of the AHE in ferromagnets, where it was derived from the interband matrix elements of the position operator in the presence of the SO coupling. More recently, the anomalous term appeared in the Lagrangian wave-packet formalism of Ref. 37, where its relation with the Berry curvature was also clearly established. In our derivation, the anomalous velocity appeared as a result of the quantum corrections in the Poisson brackets (43). Although the anomalous velocity term can be viewed as the momentum-space dual of the Lorentz force, in which the role of the magnetic field $B$ is played by the Berry curvature $B_\lambda$, this duality is not complete. The reason is that, unlike the physical magnetic field, which satisfies the Maxwell equation $\nabla \cdot B = 0$ and is therefore always source-free, the Berry field has sources – the Berry “magnetic monopoles” or “diabolical points” – at the band degeneracy points, see Sec. III B.

To conclude this section, we recall that our analysis of the classical equations of motion relies on the assumption that the SO band splitting $E_{SO}$ is much greater than the energy scales associated with the magnetic field. In the opposite limit, i.e. if $\mu_m B \sim \hbar \omega_c \gtrsim E_{SO}$, the argument that the SO coupling is not small in the semiclassical parameter (26) and can therefore be included in $\hat{H}_0$ [Eq. (33)] fails. This limit requires a completely different approach, because the inequalities (27) and (28) are violated, which means that the classical dynamics of quasiparticles can no longer be treated separately in each helicity band. The degeneracy, or near degeneracy, of the bands changes the wavefunction geometry: The Berry connection has to be generalized from the $U(1)$ case, see Eq. (11), to the $SU(2)$ case, in which both basis eigenvectors, not just their phases, can be rotated. In this case, the helicity (or the spin) becomes a dynamical variable itself, governed by an additional equation of motion.

### B. Band degeneracies as topological defects in momentum space

In this section, we study the relation between the band degeneracies and the topological features in the electronic spectrum. Let us first consider the case of an isolated point zero in the SO coupling, symmetry-imposed or accidental, at $P = P_0$. The former possibility is
realized in many noncentrosymmetric crystals, see Table I, where $P_0 = 0$. Although both the Berry connection (45) and the Berry field (46) are not defined at the degeneracy point, one can calculate the Berry flux, $\oint_S \mathbf{B}_\lambda \cdot d\mathbf{S}$, through a closed surface $S$ in the momentum space surrounding this point. It is straightforward to show that Eq. (46) can be written as

$$B_{\lambda,i} = -\frac{\lambda}{4} \sum_{jk} \sum_{abc} e_{ijk} e_{abc} \frac{\partial \hat{g}_b}{\partial P_j} \frac{\partial \hat{g}_c}{\partial P_k}, \quad (51)$$

where $\hat{g} = g/|g|$. For the Berry flux we have

$$\oint_S \mathbf{B}_\lambda \cdot d\mathbf{S} = -2\pi \lambda Q, \quad (52)$$

where

$$Q = \frac{1}{8\pi} \sum_{ijk} e_{ijk} \oint_S \hat{g} \left( \frac{\partial \hat{g}}{\partial P_j} \times \frac{\partial \hat{g}}{\partial P_k} \right) = 0, \pm 1, \pm 2, \ldots \quad (53)$$

is the degree of a mapping, $\mathbb{P} \rightarrow \hat{g}(\mathbb{P})$, of the surface $S$ (which is homotopically equivalent to a sphere $S^2$) onto the unit sphere $S^2$ corresponding to all possible directions of $\hat{g}$. Thus the Berry flux through a closed surface is a topological invariant. Using the Gauss theorem in Eq. (52), one can write the “Maxwell equation” for the Berry field: $\nabla \cdot \mathbf{B}_\lambda = 4\pi q_\lambda \delta(P - P_0)$, with the right-hand side describing a monopole at $P = P_0$, which carries the topological charge $q_\lambda = -\lambda Q/2$. Note that, comparing Eqs. (52) and (B5), one can also relate $Q$ with another topological invariant, namely the Chern number for the $\lambda$th band: $\text{Ch}_\lambda = \lambda Q$.

For example, in a nonmagnetic cubic metal with the point group $G = O$, we have $g(P) = \gamma_0 P$, see Table I. From Eq. (53) it follows that $Q = 1$ and $q_\lambda = -\lambda/2$. In general, if there is an isolated degeneracy point at $P = 0$ then the SO coupling is a linear function of the momentum near this point: $g_i(P) = \sum_j a_{ij} P_j$. While in the triclinic case, $G = C_1$, all nine coefficients here are nonzero and different, in the higher symmetry cases some of the coefficients vanish. For the zero to be isolated, the determinant of the matrix $|a_{ij}|$ must be nonzero. The degree of the mapping $\mathbb{P} \rightarrow \hat{g}(\mathbb{P})$ is given by the sign of this determinant. Therefore, the Berry field created by the band degeneracy point has the following form:

$$B_\lambda(P) = q_\lambda \frac{\hat{P}}{|P|^2}, \quad q_\lambda = -\frac{\lambda}{2} \text{sign det} |a_{ij}|. \quad (54)$$

An entirely different kind of the Berry field singularities is encountered when the SO coupling vanishes along a whole line in the momentum space. As explained in Sec. IID accidental lines of zeros are not topologically stable in three dimensions. However, the lines
of zeros listed in Table II are required by the crystal symmetry and therefore are stable, as long as the point group is not changed by a variation of the system’s parameters. Away from a band degeneracy line, $B_\lambda(P)$ is nonsingular and determined by Eq. (46). However, along the line the angles $\alpha$ and $\beta$ are not defined, and the Berry field has a singularity that originates from the term containing $\nabla P \times \nabla P\beta$. The precise form of the singularity can be found by evaluating the line integral $\Phi^B_\lambda = \oint_C A_\lambda dP$ along a closed contour $C$ around the degeneracy line. According to the definition (41), $\Phi^B_\lambda$ is nothing but the Berry phase associated with this contour.

In order to illustrate what is happening, let us look at a tetragonal crystal with $G = C_{4v}$, where the SO coupling can be written as

$$g(P) = \gamma_\perp (P_y \hat{x} - P_x \hat{y}) + \gamma_\parallel P_x P_y (P_x^2 - P_y^2), \quad (55)$$

see Table II ($\gamma_\perp$ and $\gamma_\parallel$ are constants). The SO coupling vanishes along the line $P_x = P_y = 0$. Introducing cylindrical coordinates in the momentum space: $P_x = P_\perp \cos \varphi$, $P_y = P_\perp \sin \varphi$, and $P_z$, we obtain for the Berry potential: $A_\lambda = (-1/2 + f_\lambda) \nabla P\varphi$, where

$$f_\lambda(P_\perp, P_z, \varphi) = \frac{\lambda}{2} \frac{\gamma_\parallel P_z^2 \sin 4\varphi}{\sqrt{16 \gamma_\perp^2 + \gamma_\parallel^2 P_\perp^2 P_z^2 \sin^2 4\varphi}}.$$

We draw an arbitrary closed contour $C$ and evaluate the Berry phase integral:

$$\Phi^B_\lambda = -\pi N + \tilde{\Phi}^B_\lambda(C). \quad (56)$$

The first term on the right-hand side contains only the winding number $N$ of the contour around the degeneracy line, and therefore is topologically invariant. In contrast, the second term is not topological, because it explicitly depends on the shape and size of the contour: For instance, if $N = 1$ and both $P_\perp$ and $P_z$ are single-valued functions of $\varphi$, then $\tilde{\Phi}^B_\lambda(C) = \int_0^{2\pi} f_\lambda(P_\perp(\varphi), P_z(\varphi), \varphi) d\varphi$. Considering a small contour around the degeneracy line, one can set $P_\perp \to 0$, then $\tilde{\Phi}^B_\lambda(C) \to 0$ and the remaining topological contribution means that the Berry field has a $\delta$-function singularity of the form $-\pi \delta(k_x)\delta(k_y)$.

The Berry phase becomes entirely topological in the limit of a “two-dimensional” SO coupling, mentioned in Sec. II D. In this case, $g_z(P) = 0$, and, therefore, $A_\lambda = -\nabla P\beta/2$ and

$$\Phi^B_\lambda = -\frac{1}{2} \oint_C \delta(P) = -\pi N_\beta, \quad (57)$$
where \( N_\beta \) is the winding number of the angle \( \beta(P) \) accumulated as \( P \) moves around the contour \( C \).

To summarize, the Berry field created by a line of zeros of the SO coupling contains both the topological and nontopological contributions. While the latter is given by Eq. (46), the former is the same as that of an infinitely-thin “solenoid” in the momentum space coinciding with the line of zeros. The solenoid creates a nonzero vector potential \( \mathbf{A}_\lambda(P) \) around it, which affects the Berry phase for contours enclosing the line of zeros, similarly to the Aharonov-Bohm effect. In contrast, if a band degeneracy line is present in a centrosymmetric crystal, then one can show that the Berry field still has a delta-function singularity at the line but vanishes everywhere else, i.e. the Berry field is entirely topological. The origin of the difference between the two cases can be understood using the fact that in the presence of both time reversal and inversion symmetries the band eigenstates can be chosen real. According to Eq. (42), this means that the Berry field is zero, except at such \( P \) where the eigenvectors and their derivatives are not defined, which is exactly what happens at the degeneracy line.

IV. SELECTED APPLICATIONS

A. Lifshitz-Onsager relation and de Haas-van Alphen effect

In this section we discuss manifestations of the nontrivial band topology in a noncentrosymmetric metal. Our main focus will be on the electron dynamics in the presence of a uniform applied field, in particular, on the dHvA effect. The first step is to understand how the anomalous velocity affects the cyclotron motion of the quasiparticles and also identify the invariant tori and contours in phase space required for the Bohr-Sommerfeld quantization. The starting point in the quantization procedure is the expression (39) for the action integral, which can be transformed into

\[
J = \oint_C P \, dr - e \oint_C A(r) \, dr + \hbar \oint_C \mathbf{A}_\lambda(P) \, dP, \tag{58}
\]

where \( C \) is a closed contour. The integrals here can be calculated using a straightforward generalization of the textbook argument, see, e.g., Ref. 38.

We assume a uniform applied magnetic field \( B \), choose the \( z \)-axis along the field, and set
$E = 0$. Then it follows from Eq. (50) that there are three integrals of motion:

$$I_1 = P_x + \frac{eB}{c} y, \quad I_2 = P_y - \frac{eB}{c} x, \quad I_3 = P_z,$$

in addition to the Hamiltonian $\mathcal{H}_\lambda$. Equations of motion can be transformed into the following form:

$$\frac{d\mathbf{r}}{dt} = \mathbf{V}_\lambda(\mathbf{P}), \quad \frac{d\mathbf{P}}{dt} = -\frac{e}{c} [\mathbf{V}_\lambda(\mathbf{P}) \times \mathbf{B}],$$

where

$$V_{\lambda,x} = \frac{v_{\lambda,x}}{1 + (\hbar e/c) B B_{\lambda,z}}, \quad V_{\lambda,y} = \frac{v_{\lambda,y}}{1 + (\hbar e/c) B B_{\lambda,z}}, \quad V_{\lambda,z} = v_{\lambda,z} + \frac{\hbar e}{c} B (B_{\lambda,x} v_{\lambda,x} + B_{\lambda,y} v_{\lambda,y})$$

[the singularity of $V_{\lambda,x}$ and $V_{\lambda,y}$ at $B_{\lambda,z}(P) = -c/\hbar e B$ is spurious because our results are only valid in the first order in $\hbar$]. It follows from Eq. (60) that $\dot{P} \mathbf{v}_\lambda = 0$, therefore $P_x$ and $P_y$ trace out an orbit in momentum space which is defined by the intersection of the constant-energy surface $\mathcal{H}_\lambda(\mathbf{P}) = E$ with the plane $P_z = I_3$. If the orbit is closed, then $P_x$ and $P_y$ are periodic functions of time. The corresponding real-space coordinates can be found from Eq. (59), from which it follows that $x$ and $y$ also trace out a closed orbit in the $xy$-plane, therefore the real-space trajectory is coiled around a cylinder parallel to the $z$-axis.

We choose the integration contour in Eq. (58) to coincide with the momentum space orbit, with $x$ and $y$ found from Eq. (59) and $z = \text{const}$. The first term on the right-hand side of Eq. (58) is $(2c/eB) A_\lambda$, where $A_\lambda$ the area in momentum space enclosed by the orbit. The second term is $(eB/c) A_{\lambda}^{xy}$, where $A_{\lambda}^{xy} = (c/eB)^2 A_\lambda$ is the area of the corresponding orbit in the $xy$ plane. The last integral is the Berry phase $\Phi^B_\lambda$ accumulated as the particle completes one revolution along the orbit. Collecting together all three contributions, we obtain:

$$J = \frac{c}{eB} A_\lambda + h\Phi^B_\lambda.$$

The Berry phase term represents a linear in $\hbar$ correction to the action integral. Since the Hamiltonian $\mathcal{H}_\lambda(\mathbf{P})$ also contains a quantum correction due to the magnetic moment interaction, which is given by the last term in Eq. (47), one must, for consistency, also expand the area of the orbit: $A_\lambda = A_{0,\lambda} + A_{1,\lambda} + \mathcal{O}(\hbar^2)$. The linear in $\hbar$ correction has the following form: $A_{1,\lambda} = hB \int_C (dP_\perp/v_{\lambda,\perp}) m_{\lambda,z}$, where $\mathbf{P}_\perp$ denotes the components of momentum perpendicular to $\mathbf{B}$, and $v_{\lambda,\perp} = \left| \partial \mathcal{H}_{0,\lambda} / \partial \mathbf{P}_\perp \right|$. 
In arbitrary coordinate axes, a plane perpendicular to the magnetic field is defined by the equation \( \mathbf{P} \hat{B} = P_0 \), where \( \hat{B} = \mathbf{B}/B \), and \( P_0 \) is a constant. Then \( A_{0,\lambda} \) is the area of the intersection of the plane \( \mathbf{P} \hat{B} = P_0 \) with the constant energy surface \( \mathcal{H}_{0,\lambda} = E \), where \( \mathcal{H}_{0,\lambda}(\mathbf{P}) = \varepsilon(\mathbf{P}) + \lambda |\mathbf{g}(\mathbf{P})| \), see Eq. (36). We refer to this intersection as the classical orbit \( C_\lambda(E, P_0) \). Imposing the Bohr-Sommerfeld quantization condition on the action integral (61) and neglecting the terms of the order of \( \hbar^2 \), we arrive at the following equation:

\[
\tilde{A}_\lambda(E, P_0) = 2\pi\hbar e B \left( n + \frac{1}{2} \right),
\]

(62)

which implicitly determines the quasiparticle energy levels \( E_{\lambda,n}(P_0) \) in the \( \lambda \)th band. The area of the classical orbit is modified by the quantum corrections as follows:

\[
\tilde{A}_\lambda = A_{0,\lambda} + \frac{\hbar e B}{c} (\Phi^m_\lambda + \Phi^B_\lambda),
\]

(63)

where

\[
\Phi^m_\lambda(E, P_0) = \frac{c}{e} \oint_{C_\lambda} \frac{m_\lambda(\mathbf{P}) \hat{B}}{v_{\lambda,\perp}(\mathbf{P})} dP_\perp,
\]

(64)

results from the deformation of the orbit by the interaction of the magnetic moment (49) with the applied field, and

\[
\Phi^B_\lambda(E, P_0) = \oint_{C_\lambda} \mathbf{A}_\lambda(\mathbf{P}) d\mathbf{P},
\]

(65)

is the Berry phase associated with the orbit. Thus we have reproduced the Lifshitz-Onsager relation, with \( \gamma_\lambda = 1/2 - (\Phi^m_\lambda + \Phi^B_\lambda)/2\pi \), the deviation from the universal value 1/2 being due to the quantum corrections to semiclassical dynamics.

The orbital quantization of the energy levels leads to a variety of magnetooscillation phenomena, including the dHvA effect. The oscillatory behaviour of the magnetization as a function of the applied field is described by the Lifshitz-Kosevich formula, which relates the dHvA frequencies to the extremal, with respect to \( P_0 \), cross-sections of the Fermi surface. In our case it follows from the quantization condition (62) that, instead of the usual geometrical area of the cross-section, one must use the modified area given by Eq. (63). Including both helicity bands, we obtain the oscillating contribution to the magnetization along the field:

\[
M = \sum_\lambda \sum_{ex} M_{\lambda,ex}^x \sin \left( \frac{2\pi F_{\lambda,ex}^x}{B} \pm \frac{\pi}{4} \right),
\]

(66)

where the summation goes over all the extremal cross-sections, \( M_{\lambda,ex}^x \) are the amplitudes of the oscillations, and the plus and minus signs in the phase shifts correspond to minimum and
maximum cross-sectional areas, respectively, see Ref. 38. The frequencies of the oscillations are given by $F^{ex}_\lambda = \frac{c}{2\pi\hbar e} \tilde{A}^{ex}_\lambda$, where $\tilde{A}^{ex}_\lambda$ is the value of expression (63) at the extremum, with $E = \epsilon_F$. The extremum can be shifted away from its classical position (which corresponds to the extremum of $A_{0,\lambda}$) due to $\Phi^m_\lambda$ and $\Phi^B_\lambda$, but this effect can be neglected, since it produces a correction to the area that is quadratic in the semiclassical parameter. We note that Eq. (66) is approximate: In addition to the fundamental harmonics, the observed dHvA signal also contains higher harmonics with the frequencies given by integer multiples of $F^{ex}_\lambda$.

As a simple illustration, let us consider a nonmagnetic cubic metal with $G = O$. Real-life examples of this symmetry include the Li$_2$(Pd$_{1-x}$Pt$_x$)$_3$B family of materials. We assume a parabolic band, $\epsilon(p) = p^2/2m^*$, with the effective mass $m^*$, and use $g(P) = \gamma_0 P$ for the SO coupling, see Table I. The Fermi surfaces are spheres of radii $P_{F,\lambda}$, and the extremal classical orbits are two great circles perpendicular to the field, therefore $A^{ex}_{0,\lambda} = \pi P_{F,\lambda}^2$. Since the extremum is in fact the maximum, one must use the negative sign in Eq. (66).

There is an isolated band degeneracy at $P = 0$, which creates a monopole-like Berry field $B_\lambda(P) = -\left(\lambda/2P_{F,\lambda}^2\right) \hat{P}$, see Eq. (54). From Eq. (49) it follows that $m_\lambda \hat{B} = 0$ at the orbit, therefore $\Phi^m_\lambda = 0$. The Berry phase is nonzero and given by $\Phi^B_\lambda = -\lambda \pi$, which yields a field-dependent correction to the dHvA frequencies: $F^{ex}_\lambda = cP_{F,\lambda}^2/2\hbar e - \lambda B/2$. From Eq. (66) we obtain:

$$M = -\sum_\lambda M_\lambda \sin \left(\frac{\pi c P_{F,\lambda}^2}{\hbar e B} - \frac{\pi}{4}\right),$$

i.e. the phase of the magnetization oscillations is shifted by 180° compared to the Lifshitz-Kosevich result without the quantum corrections. Such a phase shift can be measured in the dHvA experiments. For the Lifshitz-Onsager parameter, we have $\gamma = 0$ (the values $\gamma = 0$ and $\gamma = 1$ are equivalent). One can expect that higher orders in the semiclassical expansion will produce corrections of the order of $B^2$ to the dHvA frequencies, which will give rise to a magnetic field dependence of the phase shifts in the Lifshitz-Kosevich formula (one such correction was discussed in Ref. 61).

Previous works on the semiclassical electron dynamics in magnetic field have focused almost exclusively on the centrosymmetric case, where one can show that Lifshitz-Onsager’s $\gamma$ also differs from 1/2 in the general case, i.e. in the presence of both the SO coupling and the Zeeman interaction. The deviation is non-universal in the sense that,
similar to our Eqs. (64) and (65), it depends on the details of the classical orbit, and can be interpreted in terms of the evolution of a classical spin vector along the orbit. We recall that, in the centrosymmetric case, the SO coupling does not remove the spin degeneracy of the bands, therefore the quasiparticle equations of motion must take into account the transitions between the states with opposite spin projections. This is also true in a “weakly-noncentrosymmetric” case, when the SO band splitting is small compared to the energy scales associated with the external magnetic field, see the last paragraph of Sec. III A.

We would like to mention also the studies of magnetic oscillation phenomena using the Gutzwiller trace formula, which must be modified in the presence of the SO coupling to include additional factors describing the classical spin evolution.[57, 62]

Interestingly, $\gamma$ is not necessarily equal to $1/2$, even when the electron spin is completely neglected, which formally corresponds to setting $g(p) = 0$ and $\mu_m = 0$. In this case, the magnetic moment vanishes and the correction to $\gamma$ is entirely due to the Berry phase, see Ref. 34 and especially Ref. 37, where the spinless limit was studied using the wave-packet formalism. As mentioned in the end of Sec. III D, the Berry phase is either $\pm \pi$ or 0, depending on whether or not the orbit encloses a band degeneracy line in the Brillouin zone, therefore in the spinless case there are only two possibilities: $\gamma = 0$ or $\gamma = 1/2$ (Ref. 41).

B. Magnetic crystals: Anomalous Hall effect

Another possible application of the formalism developed in Sec. III is the AHE, which is the appearance of a transverse component of the electric current in ferromagnetic substances, even in the absence of external magnetic field (for recent reviews see, e.g., Refs. 63 and 64). Semiclassical theory of this phenomenon can be obtained by setting $B = 0$ in Eq. (50), which yields:

$$\frac{dr}{dt} = v_\lambda(p) + e\hbar E \times B_\lambda(p).$$

(68)

We assume a uniform electric field and neglect the internal induction due to magnetization, which is known to be too small to account for the AHE. The “intrinsic” Hall current originates from the second term in Eq. (68) and can be obtained by adding the contributions from both helicity bands:

$$j_H = -e^2\hbar \sum_\lambda \sum_p \{E \times B_\lambda(p)\} f_\lambda(p),$$

(69)
where \( f_\lambda(p) = [e^{i\xi_\lambda(p)} + 1]^{-1} \) is the quasiparticle distribution function \((\beta = 1/k_B T)\), and 
\[ \xi_\lambda(P) = \varepsilon(P) + \lambda |g(P)| - \varepsilon_F. \]
It follows from Eq. (69) that the anomalous Hall current vanishes in the absence of time-reversal symmetry breaking, i.e. at \( h = 0 \), in which case \( B_\lambda \) is odd in \( p \) (see Sec. III A), while \( f_\lambda \) is even. We see that the intrinsic AHE is essentially an equilibrium phenomenon, which is related to the Berry curvature of the band wavefunctions, see Refs. 23, 24, and 65. Moreover, using the expression \( B_\lambda = \nabla_p \times A_\lambda \) and integrating Eq. (69) by parts, one can show that \( j_H \) is determined by the quasiparticle properties near the Fermi surface. This means that not only the semiclassical description of the AHE is legitimate, but it can also be extended to interacting systems using the standard Fermi-liquid theory arguments. [25]

In two dimensions, one obtains from Eq. (69) the Hall conductivity in the form
\[ \sigma_{xy} = -(e^2/2\pi h) \int_{FBZ} dp_x dp_y \sum_\lambda B_{\lambda,z} f_\lambda, \]
where \( h = 2\pi \hbar \) and the momentum integration is performed over the first Brillouin zone. Using Eq. (51) this can be written as
\[ \sigma_{xy} = \frac{e^2}{h} \frac{1}{4\pi} \int_{FBZ} dp_x dp_y \hat{g} \left( \frac{\partial \hat{g}}{\partial p_x} \times \frac{\partial \hat{g}}{\partial p_y} \right) \left[ f_+(p) - f_-(p) \right]. \] (70)
The last expression takes a particularly appealing form in the case of a magnetic insulator, which is realized when the chemical potential lies in the gap between the “+” and “−” bands. The band gap is given by \( \min[\varepsilon(p) + |g(p)|] - \max[\varepsilon(p) - |g(p)|] \), which vanishes in the nonmagnetic case due to the mandatory zeros of the SO coupling, see Sec. II D. At zero temperature, Eq. (70) becomes
\[ \sigma_{xy} = -\frac{e^2}{h} \frac{1}{4\pi} \int_{FBZ} dp_x dp_y \hat{g} \left( \frac{\partial \hat{g}}{\partial p_x} \times \frac{\partial \hat{g}}{\partial p_y} \right) = -\frac{e^2}{h} Q, \] (71)
where \( Q = 0, \pm 1, \ldots \) is the degree of a mapping of the Brillouin zone (a torus) onto a unit sphere \( S^2 \), cf. Eq. (53). Thus we come to the conclusion that the anomalous Hall conductivity in a two-dimensional ferromagnetic noncentrosymmetric insulator is quantized, in agreement with the result of Ref. 66, which was obtained by a Kubo formula calculation. This phenomenon is similar to the integer quantum Hall effect in an external magnetic field,[21] both originating from the quantization of the Berry flux through a two-dimensional Brillouin zone.

We would like to note that the simple semiclassical picture of the AHE apparently fails in a perfect lattice,[67] where, according to the second of Eq. (50), we have \( p(t) = p(0) - eEt \). Due to the crystal periodicity, both \( v_\lambda \) and \( B_\lambda \) are periodic functions of \( p \), which means that
the quasiparticle’s velocity $\dot{r}$ is a periodic, or at least bounded, function of time. The quasiparticle oscillates in space and therefore cannot carry any net electric current. However, this argument against the intrinsic AHE is not fully satisfactory, because the linearly increasing momentum, when mapped back into the first Brillouin zone, can eventually pass arbitrarily close to a band degeneracy, where the anomalous velocity is singular and the semiclassical description does not work. In addition, the case of a perfectly periodic crystal is rather unphysical, because of various scattering processes always present in real materials. More detailed discussion of the AHE in ferromagnetic noncentrosymmetric metals, which should include the scattering effects, is beyond the scope of this paper.

V. CONCLUSIONS

The symmetric and antisymmetric contributions to the electron-lattice SO coupling in crystals without inversion symmetry play qualitatively different roles. While the former just replaces spin with pseudospin, preserving the twofold degeneracy of the bands, the latter removes the band degeneracy almost everywhere in the Brillouin zone and creates a nonzero Berry curvature of the resulting helicity bands. In contrast to the centrosymmetric case, there are always remaining band degeneracies in each band. The anisotropy of the SO coupling, in particular the type and location of the band degeneracies, is determined by the crystal symmetry, see Table I.

Using a reduced one-band model of the antisymmetric SO coupling (the generalized Rashba model), we derived the semiclassical equations of motion of the quasiparticles in the helicity bands, taking into account all effects associated with the electron spin. We have found two distinct types of quantum corrections to the semiclassical dynamics: One, which is entirely due to the Berry curvature of the bands, makes the Poisson brackets noncanonical and results in the anomalous velocity term in the equations of motion. The other, which appears directly in the classical Hamiltonian, describes the interaction of the magnetic moment of the band quasiparticles with the applied magnetic field. The magnetic moment contains both spin and orbital contributions mixed by the SO coupling and is also affected by the Berry curvature. Both types of the quantum corrections modify the Bohr-Sommerfeld quantization condition, which makes them observable, e.g., in the dHvA effect.

We have considered only the case of noninteracting electrons in a normal noncentrosym-
metric metal. One can expect that the nontrivial topology of the band wavefunctions should also affect the properties of interacting systems. Although there have been some interesting recent developments, see Refs. 25, 68, 69, this subject remains largely unexplored.

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APPENDIX A: TRANSFORMATION PROPERTIES OF QUANTUM STATES AND OPERATORS

We adopt the convention that a symmetry transformation, either a point group operation \( g \) or time reversal \( K \), changes the physical state of the system, not the coordinate axes. Under a proper rotation \( g = R \), the position vector \( \mathbf{r} \) is transformed into \( \mathbf{r}' = R \mathbf{r} \), where \( R \equiv D^{(1)}(R) \) is the rotation matrix in the spin-1 representation. We recall that the rotation about a direction \( \mathbf{n} \) by an angle \( \theta \) (\( \theta \) is positive for a counterclockwise rotation) in the spin-\( J \) representation is described by the matrix \( D^{(J)}(R) = \exp(-i \theta \mathbf{n} \cdot \hat{J}) \), where \( \hat{J} \) are the generators of rotations. Under an improper operation \( g = IR \), which is represented as a product of a rotation \( R \) and inversion \( I \), we have \( \mathbf{r} \rightarrow \mathbf{r}' = -R \mathbf{r} \). In particular, for spin-1/2 particles, we have \( D^{(1/2)}(g) = e^{-i\theta(n \cdot \mathbf{\sigma})/2} \) for both \( g = R \) and \( g = IR \), since inversion does not affect the spin degrees of freedom.

Let us consider non-interacting electrons in an ideal crystal lattice, see Eq. (1). The action of the point group and time reversal operations on spinor wavefunctions is discussed, e.g., in Ref. 70. Neglecting the SO coupling and omitting the orbital band index, the eigenstates are the Bloch spinors \( \langle \mathbf{r} \sigma | s \rangle \equiv \psi_{k,s}(\mathbf{r}, \sigma) = \Phi_k(\mathbf{r}) \delta_{ss'} \), where \( \Phi_k(\mathbf{r}) = V^{-1/2} \varphi_k(\mathbf{r}) e^{ik\mathbf{r}} \), see Eq. (2). Under a point group operation \( g \), these transform into

\[
g \psi_{k,s}(\mathbf{r}, \sigma) = \sum_{\sigma'} D_{\sigma \sigma'}^{(1/2)}(g) \psi_{k,s}(g^{-1} \mathbf{r}, \sigma') = D_{ss'}^{(1/2)}(g) \Phi_k(g^{-1} \mathbf{r}) = \sum_{s'} \psi_{gk,s'}(\mathbf{r}, \sigma) D_{ss'}^{(1/2)}(g).
\]

(A1)
Here we used the fact that $\Phi_k^*(g^{-1}r)$ corresponds to the wave vector $gk$. Under time reversal,

$$K\psi_{k,s}(r,\sigma) = \sum_{\sigma'} (-i\sigma_2)_{\sigma\sigma'} \psi_{k,s}^*(r,\sigma') = (-i\sigma_2)_{ss'} \Phi_k^*(r) = \sum_{s'} (i\sigma_2)_{ss'} \psi_{-k,s'},$$

(A2)

because $\Phi_k^*(r)$ corresponds to the wave vector $-k$.

Thus we obtain that the Bloch eigenstates transform under the point group operations and time reversal as follows:

$$g|ks\rangle = \sum_{s'} |gk,s'\rangle D_{\frac{1}{2}}(g), \quad K(f|ks\rangle) = f^* \sum_{s'} (i\sigma_2)_{ss'} | -k,s'\rangle.$$  (A3)

We included a constant $f$ in the second of these expressions to highlight the antilinearity of the time reversal operation. The transformation rules for the second quantization operators follow immediately from Eq. (A3), if one views the Bloch eigenstates as vectors in the Fock space: $|ks\rangle = a_{ks}^\dagger |0\rangle$, where $|0\rangle$ is the vacuum state, and assumes that the vacuum is invariant under all symmetry operations. [71]

**APPENDIX B: BAND-PROJECTED POSITION OPERATORS**

In this Appendix we discuss the physical origin of the noncanonical Poisson brackets in the semiclassical dynamics of quasiparticles in a given helicity band. We neglect external fields and focus on the first of the expressions (43). The Poisson brackets can be obtained in the classical limit from the commutator of the “band-projected” position operators $\hat{r}_\lambda = \hat{\Pi}_\lambda \hat{r} \hat{\Pi}_\lambda$, where $\hat{r}$ is the usual position operator ($\hat{r} = i\nabla_k$ in the $k$-representation), and $\hat{\Pi}_\lambda (k) \equiv |k\lambda\rangle \langle k\lambda|$ are the operators projecting onto the $\lambda$th band. Here and below no summation over repeated band indices is assumed. Since $\hat{\Pi}_\lambda^2 = \hat{\Pi}_\lambda$, we obtain:

$$\hat{r}_\lambda = i\hat{\Pi}_\lambda \frac{\partial}{\partial k} \hat{\Pi}_\lambda = i\hat{\Pi}_\lambda \frac{\partial}{\partial k} + \hat{\Omega}_\lambda, \quad \hat{\Omega}_\lambda = i\hat{\Pi}_\lambda \frac{\partial \hat{\Pi}_\lambda}{\partial k}.$$  (B1)

The band-projected position operators are $U(1)$ gauge covariant, in the following sense: An arbitrary phase rotation of the wavefunctions in the reciprocal space, $\psi(k) \to e^{i\chi(k)} \psi(k)$, leaves the matrix elements of $\hat{r}_\lambda$ invariant, if it is accompanied by changing $\hat{\Omega}_\lambda \to \hat{\Omega}_\lambda + (\nabla_k \chi) \hat{\Pi}_\lambda$. This variation of $\hat{\Omega}_\lambda$ can be achieved by redefining the phases of the eigenstates: $|k\lambda\rangle \to e^{i\theta_\lambda(k)} |k\lambda\rangle$, with $\theta_\lambda(k) = -\chi(k)$, which does not affect $\hat{\Pi}_\lambda$.

Using the fact that $\hat{\Pi}_\lambda (\nabla \hat{\Omega}_\lambda) \hat{\Pi}_\lambda = 0$, the commutator of the band-projected positions can be represented as follows: $[\hat{r}_{\lambda,i}, \hat{r}_{\lambda,j}] = i\hat{\Pi}_\lambda (\nabla_i \hat{\Omega}_{\lambda,j} - \nabla_j \hat{\Omega}_{\lambda,i})$. It is diagonal both in the
wave vector $k$ and the helicity $\lambda$, with the matrix elements given by

$$
\langle k\lambda | [\hat{r}_{\lambda,i}, \hat{r}_{\lambda,j}] | k\lambda \rangle = \text{tr} \left( \hat{\Pi}_\lambda \hat{\Pi}_\lambda \frac{\partial \hat{\Pi}_\lambda}{\partial k_j} - \frac{\partial \hat{\Pi}_\lambda}{\partial k_i} \hat{\Pi}_\lambda \frac{\partial \hat{\Pi}_\lambda}{\partial k_i} \right). \quad (B2)
$$

In the spin (or pseudospin) representation, the band projection operators have the form

$$
\Pi_{\lambda,\alpha\beta}(k) = u_{\alpha\lambda}(k) u_{\beta\lambda}(k),
$$

where the unitary matrix $\hat{u}(k)$ is given by Eq. (21). Inserting this in Eq. (B2), we obtain:

$$
\langle k\lambda | [\hat{r}_{\lambda,i}, \hat{r}_{\lambda,j}] | k\lambda \rangle = -\sum_{\alpha} \left( \frac{\partial u^*_{\alpha\lambda}}{\partial k_i} \frac{\partial u_{\alpha\lambda}}{\partial k_j} - \frac{\partial u^*_{\alpha\lambda}}{\partial k_j} \frac{\partial u_{\alpha\lambda}}{\partial k_i} \right). \quad (B3)
$$

In the classical limit, the commutator is replaced by the Poisson bracket: $[\hat{r}_{\lambda,i}, \hat{r}_{\lambda,j}] \to i\hbar \{r_{\lambda,i}, r_{\lambda,j}\}$. Expressing the derivatives in Eq. (B3) in terms of the canonical momentum $p = \hbar k$ and introducing the eigenvectors $\tau_{\lambda}$, such that $\tau_{\lambda,\alpha}(p) = u_{\alpha\lambda}(p/\hbar)$, we arrive at the following expression:

$$
\{r_i, r_j\} = i\hbar \left( \frac{\partial \tau^*_{\lambda}}{\partial p_i} \frac{\partial \tau_{\lambda}}{\partial p_j} - \frac{\partial \tau^*_{\lambda}}{\partial p_j} \frac{\partial \tau_{\lambda}}{\partial p_i} \right) = \hbar F_{\lambda,ij}(p), \quad (B4)
$$

where $F_{\lambda,ij}$ is the Berry curvature tensor in the momentum space, defined by Eq. (42). Thus we have recovered the first of Eqs. (43).

It is instructive also to interpret our results using the language of differential geometry. The antisymmetric tensor $F_{\lambda,ij}$ can be used to define the Berry curvature 2-form in the $\lambda$th band as follows:

$$
\omega_{B,\lambda} = (1/2) \sum_{ij} F_{\lambda,ij}(p) dp_i \wedge dp_j,
$$

where $dp_i \wedge dp_j = -dp_j \wedge dp_i$ is the wedge product. Comparing the right-hand sides of Eqs. (B2) and (B4) and expressing the band projection operators in terms of $p$, we obtain:

$$
\omega_{B,\lambda} = i \sum_{ij} \text{tr} \left( \hat{\Pi}_\lambda \frac{\partial \hat{\Pi}_\lambda}{\partial p_i} \frac{\partial \hat{\Pi}_\lambda}{\partial p_j} \right) dp_i \wedge dp_j = i \text{tr} \left( \hat{\Pi}_\lambda d\hat{\Pi}_\lambda \wedge d\hat{\Pi}_\lambda \right).
$$

In these notations the flux of the Berry field through a closed surface $S$ in the momentum space is given by the following expression:

$$
\oint_S B_{\lambda} \cdot dS = \int_S \omega_{B,\lambda} = -2\pi \left[ \frac{1}{2\pi i} \int_S \text{tr} \left( \hat{\Pi}_\lambda d\hat{\Pi}_\lambda \wedge d\hat{\Pi}_\lambda \right) \right] = -2\pi \text{Ch}_\lambda. \quad (B5)
$$

The expression in the square brackets is an integer, which is known as the (first) Chern number for the $\lambda$th band. The Chern numbers are probably best known in condensed matter physics for the role they play in explaining the integer quantum Hall effect.
In Eq. (B5) we used the expression for the Chern numbers in terms of the band projection operators from Ref. 72.

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