Geometric (or Berry) phase has become a powerful tool for analysis of waves in periodic systems, especially in crystals. Wavevector $\vec{k}$ provides a space in which adiabatic evolution of wavefunctions $\psi_n(\vec{k})$ can be studied. Singular behavior occurs at band degeneracies where energies $\epsilon_1(\vec{k}) = \epsilon_2(\vec{k})$ are equal. In crystals with inversion symmetry, ignoring spin-orbit interactions, degeneracies occur along closed lines in $\vec{k}$-space. The periodic part $u_n(\vec{k}, \vec{r}) = \exp(-i\vec{k} \cdot \vec{r})\psi_n(\vec{k}, \vec{r})$ of $\psi$ is an eigenstate of $H(\vec{k}) = (\vec{p} + \hbar \vec{V})^2/2m + V(\vec{r})$. Let the wavevector $\vec{k}(t)$ be given a time evolution which takes it on the circuit $C$, with $\vec{k}(T) = \vec{k}(0)$. Now suppose that wavefunction evolution is determined by the time-dependent Schrödinger equation with the time-dependent Hamiltonian $H(\vec{k}(t))$. The time-evolution is assumed adiabatic, namely $u_n(\vec{k}, \vec{r}, t) \propto u_n(\vec{k}(t), \vec{r})$. Berry’s argument shows that $u_n(\vec{k}, \vec{r}, T)$ differs from $u_n(\vec{k}, \vec{r}, 0)$ by the factor $\exp[i\gamma(C, T)]$, where the phase $\gamma(C, T)$ has two parts, $\gamma(C) + \gamma(T)$. The dynamical part $\gamma(T) = -\int_0^T dt\epsilon_n(\vec{k}(t))/\hbar$ depends on the time elapsed, and the geometric part

$$\gamma(C) = i \oint_C d\vec{k} \cdot \int d\vec{r} u_n^{*} \vec{\nabla}_k u_n$$

(1)

is invariant and intrinsic to the circuit and the band properties. In particular, $\gamma(C) = \pm \pi$ if $C$ encloses one (or an odd number) of degeneracy lines. This change of wavefunction sign is familiar from other problems where a circuit of adiabatic evolution surrounds a conical intersection. Direct evaluation of Eq. (1) is problematic. Wavefunctions must be continuous and single-valued.

Although gauge invariance is not evident in Eq. (1), Berry gave also an alternate form, for a 3-dimensional parameter space $\vec{k}$, as the flux through a surface $S$ (bounded by $C$) of a vector $\vec{V}_n$.

$$\gamma(C) = -\int_S d\vec{S}_k \cdot \vec{V}_n$$

(2)

$$\vec{V}_n = \text{Im} \sum_m \frac{\langle m | \vec{\nabla}_k H | m \rangle \times \langle m | \vec{\nabla}_k H | n \rangle}{\epsilon_m(\vec{k}) - \epsilon_n(\vec{k})}$$

(3)

The gauge invariance of this vector is evident. Conditions of continuity and single-valuedness of wavefunctions are no longer required. If the circuit surrounds a singularity described by a $2 \times 2$ effective Hamiltonian, then the flux equals half the solid angle $\Omega(C)$ subtended in an appropriate scaled space by the circuit as seen from the point of singularity. The appropriate scaled space is the one in which the $2 \times 2$ Hamiltonian for states near the conical intersection has the form $H_{\text{eff}} = \vec{R} \cdot \vec{\sigma}$ in terms of scaled coordinates $\vec{R} = (X, Y, Z)$ and Pauli matrices $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. This method will be used twice in this paper. The eigenvalues are $\pm \rho \rho = \rho, \rho R$, where the quantum number $\rho = \pm 1$ is introduced as a branch index. The geometric phase is then $\gamma(C) = -\rho \Omega(C)/2$.

Mikitik and Sharma provide convincing evidence that the geometric phase $\pm \pi$ is seen experimentally as a shift in the semiclassical quantization condition determining the de Haas-van Alphen oscillations. An extreme experimental case is the shifted quantum Hall oscillations originating from orbits near the “Dirac points” in graphene. The shifts of quantization condition occur for electron orbits (in a $\vec{B}$-field) which surround a degeneracy line (or point, for graphene.) They also argue that spin-orbit effects can mostly be ignored. This is correct for lighter elements with spin-orbit strength $\xi/\Delta \ll 1$, $\Delta$ being any other relevant electron scale such as a band gap. However, the mathematics and the corrections need elucidation. Spin-orbit coupling destroys band degeneracy lines. It is not evident what happens to the geometric phase of $\pm \pi$.

To see the effect of spin-orbit interactions, add to $H(\vec{k})$ the piece $H_{\text{SO}} = (\vec{\sigma}/4m^2c^2) \cdot \vec{\nabla} V \times (\vec{p} + \hbar \vec{k})$. Choose some point $\vec{k}^*$ of accidental degeneracy, and find energies and eigenstates at nearby $\vec{k}$-points using degenerate $\vec{k} \cdot \vec{p}$ perturbation theory. For notational simplicity, $\vec{k}^*$ is the temporary origin of $\vec{k}$. The degenerate basis functions $|1\rangle$ and $|2\rangle$ are the periodic parts $u_1$ and $u_2$ at $\vec{k} = \vec{k}^*$. A phase convention is needed; the coefficients $C_{G}$ of the expansion $u(\vec{r}) = \sum C_{G} \exp(iG \cdot \vec{r})$ are chosen real. This requires inversion symmetry, which is here-mentioned. Each state has two spin orientations, so
the effective Hamiltonian matrix is 4 × 4, with the form
\[ h \mathbf{H}_{\text{eff}} = \begin{pmatrix} h\vec{k} \cdot \vec{v}_1 & h\vec{k} \cdot \vec{v}_1 - i\xi \cdot \vec{\sigma} \\ h\vec{k} \cdot \vec{v}_1 + i\xi \cdot \vec{\sigma} & -h\vec{k} \cdot \vec{v}_2 \end{pmatrix} \]

where \( \vec{1} \) and \( \vec{\sigma} \) are 2 × 2 matrices in spin space. Terms proportional to the 4 × 4 unit matrix do not mix or split the states and are omitted. The vector \( \vec{v}_n \) is \( (\vec{v}_1 - \vec{v}_2)/2 \), where \( \vec{v}_n \) is the band velocity \( \vec{V}_k n / \hbar \) at the degeneracy \( k^* \). The vector \( \vec{v}_b \) is the off-diagonal term \((2|\vec{p}|/m1)\), which is purely real since \( C_G \) is real. The solid angle is \( 4/\pi V^2 \), where \( \hat{v}_a, \hat{v}_b, \) and \( \xi \) determine the bands near \( k^* \). The vector \( \xi \) is a close analog to angular momentum. Consider a system with two degenerate \( p \)-states \( |x\rangle \) and \(|y\rangle \).

The angular momentum operator \( \vec{L} \) has an imaginary off-diagonal element. The mixed states \(|x\rangle \pm i|y\rangle \) are eigenstates of \( \vec{L} \) with \( \langle \vec{L} \rangle = \pm m\hbar \xi \). The magnitude \( m \) deviates from 1 if the point symmetry is less than spherical. The vector \( \xi \) will be called the “orbit moment.”

First suppose that \( \xi = 0 \). Since \( \vec{v}_a \) and \( \vec{v}_b \) are not generally co-linear, they define a direction of \( \vec{k} \), namely \( \vec{v}_a \times \vec{v}_b \), along which \( \mathbf{H}_{\text{eff}} = 0 \). This is the direction of the line of degeneracy. After allowing \( \xi \neq 0 \), eigenvalues of Eq. (4) are \( \pm \lambda \) where
\[ \lambda = \sqrt{\kappa_a^2 + \kappa_b^2 + \xi^2} \]

with \( \kappa_a = h\vec{k} \cdot \vec{v}_a \), \( \kappa_b = h\vec{k} \cdot \vec{v}_b \), and \( \xi = |\xi| \). Each eigenvalue belongs to a Kramers doublet of two opposite spin states. The original degeneracy (without spin-orbit interaction) of 2 (neglecting spin) or 4 (including spin) is lifted everywhere unless \( \xi = 0 \). This should happen only at isolated points in the Brillouin zone, not coinciding with degeneracy lines \( k^* \). No accidental degeneracies remain, but Kramers degeneracy occurs everywhere. Bands near \( k^* \) are shown in Fig. 1.

The geometric phase under consideration involves a circuit \( C(\vec{k}) \) surrounding the \( \vec{k}^* \) line. A circular path in two-dimensional \((\kappa_a, \kappa_b)\)-space, namely \( C = (\kappa \cos \phi, \kappa \sin \phi) \), \( 0 \to \phi \to 2\pi \) is the simplest realization. To calculate \( \gamma(C) \), separate Eq. (4) into two similar 2 × 2 submatrices by choosing basis states with spins polarized along \( \xi \), which will be used as the z-axis of spin space. The submatrices are
\[ \mathbf{H}_{\text{eff}} = \begin{pmatrix} \kappa_a & i\xi \\ \kappa_b + i\xi & -\kappa_a \end{pmatrix} \]

where the upper sign goes with spin up, \( \sigma_z = 1 \).

The circuit can now be considered as a path \( C(\vec{\lambda}) \) in a 3-d \( \vec{\lambda} \)-space, where \( (\lambda_x, \lambda_y, \lambda_z) = (\kappa_b, \sigma_z \xi, \kappa_a) \). On this circuit, \( \lambda, \kappa \), and \( \xi \) are all constant. The effective Hamiltonian has the desired scaled form. The solid angle is \( \sigma_2 \pi (1 - \xi/\lambda) \), so the geometric phase is
\[ \gamma(C) = - (\Lambda_2 \sigma_2) \pi (1 - \xi/\lambda) \]

where \( \Lambda_2 = \pm 1 \) is the branch index. This is one of the two main results of this paper. It shows how spin-orbit splitting destroys the simple phase of \( \pm \pi \) when the circuit has such a small radius that \( \xi \sim \lambda \). If spin-orbit interaction is weak, it does not need a large orbit to have \( \xi/\lambda \ll 1 \) and approach the full simple phase of \( \pm \pi \).

This is not the full story. The choice to evolve at fixed \( \sigma_z \) was arbitrary. The states of Kramers doublets can be mixed by arbitrary unitary transformations. Evolution of a doublet around a circuit introduces not a simple geometric phase, but a unitary matrix. The \( \gamma(C) \) phases just computed are actually the diagonal elements \( \exp(\pm i\gamma(C)) \) of a 2 × 2 unitary matrix in the representation with spin quantized along \( \xi \). It will emerge below that this is indeed the correct adiabatic evolution of the Kramers doublet when an small magnetic field is imposed along the \( \xi \) direction.

Berry’s original argument assumed that \( \mathcal{H} \) had a discrete spectrum along \( \xi \). There is a physically natural way to retain this. Magnetic fields present in experiment since they are used to cause cyclic evolution in \( \vec{k} \)-space. Magnetic fields also lift Kramers degeneracy. The simplest theoretical device is to add to \( \mathbf{H}_{\text{eff}} \) a Zeeman term \( \mathcal{H}_Z = -\vec{B} \cdot \vec{\sigma} \) coupling only to spin.

To proceed further, an explicit representation of eigenstates is needed. Eigenstates of the effective Hamiltonian \( \mathbf{H}_\pm \), labeled by energy \( \pm \lambda \) and \( \sigma_z = \pm 1 \), are chosen as
\[ |s\rangle = | -\lambda, \uparrow \rangle = \frac{1}{n} \left( -\kappa_b + i\xi \right) \begin{pmatrix} \kappa_a + \lambda \\ \kappa_a - \lambda \end{pmatrix} \otimes | \uparrow \rangle \]
\[ |t\rangle = | -\lambda, \downarrow \rangle = \frac{1}{n} \left( -\kappa_b - i\xi \right) \begin{pmatrix} \kappa_a + \lambda \\ \kappa_a - \lambda \end{pmatrix} \otimes | \downarrow \rangle \]
\[ |u\rangle = | +\lambda, \uparrow \rangle = \frac{1}{n} \left( \kappa_a + \lambda \right) \begin{pmatrix} \kappa_a + \lambda \\ \kappa_a - \lambda \end{pmatrix} \otimes | \uparrow \rangle \]

![FIG. 1: Energy versus |\vec{k}| near the degeneracy point.](image)
\[ |v\rangle = \begin{cases} + |λ, l\rangle = \frac{1}{n} \left( \frac{κ_a + λ}{κ_b - iξ} \right) \otimes | \downarrow \rangle. \end{cases} \] (11)

These are written as direct product of spatial times spin two-vectors. The normalization is \( n = \sqrt{2(λ + κ_a)} \). As long as \( ξ \) is non-zero, \( 1/n \) is non-singular and these are smooth, single-valued functions of \( (κ_a, κ_b) \), unique except for an arbitrary overall phase, which cannot alter \( γ(C) \).

The lower Kramers doublet \( |s\rangle, |t\rangle \) has “orbit moments” \( \langle i\vec{V} \times \vec{p}/4m^2c^2 |i\rangle = ±(ξ/λ)\vec{ξ} \) oriented antiparallel to spin, while the upper Kramers doublet \( |u\rangle, |v\rangle \) has identical orbit moments except oriented parallel to spin.

Now the Zeeman term is added. Diamagnetic coupling is neglected. Without loss of generality, the part of the field \( \vec{B} = \frac{b}{μB} \) perpendicular to \( ξ \) can be used to define the \( x \) direction of spin. The total Hamiltonian in the basis \( |s\rangle, |t\rangle, |u\rangle, |v\rangle \) is

\[
H_{\text{tot}} = -\left( \begin{array}{cccc}
λ + b_z & iξb_x e^{iω} & 0 & 0 \\
ξb_x e^{-iω} & λ - b_z & -iξb_x & 0 \\
0 & iξb_x & λ + b_z & ξb_x e^{iω} \\
-iξb_x & 0 & ξb_x e^{-iω} & λ - b_z
\end{array} \right)
\] (12)

The factor \( (κ/λ) \exp(iω) = \langle s | σ_z | t \rangle \) introduces the new angle \( ω \)

\[
e^{iω} = \frac{λ - iκb_z}{κ(λ + κ_a)}.
\] (13)

As the circuit \( C \) is followed (\( φ \) going from 0 to 2π, with \( ξ, κ, λ \) constant), \( ω \) also evolves from 0 to 2π.

If the field \( b \) is along \( z \), the upper and lower Kramers doublets are not coupled. The degeneracy is lifted everywhere, and adiabatic evolution proceeds smoothly on the resulting non-degenerate states, yielding the phases \( γ(C) \) of Eq. (7). The previous discussion was correct. The result \( 7 \) can also be obtained directly from Eq. (11) using Eqs. (8) (10) (11). For fields perpendicular to \( z \), there is both intra- and inter-doublet spin mixing, according to Eq. (12). To first order, since \( b \ll λ \), inter-doublet mixing terms \( ±iξb_x / λ \) can be neglected, giving 2 × 2 effective Hamiltonian matrices, of the form

\[
H_{\text{eff}}(b) = λ_z λ_t \hat{I} - \left( \begin{array}{cc}
b_z & \xi b_x e^{iλ_1 ω} \\
\frac{1}{2}b_x e^{-iλ_1 ω} & -b_z
\end{array} \right)
\] (14)

The eigenvalues are

\[
\pm λ ± μ \quad \text{where} \quad μ^2 = b_z^2 + \frac{κ^2}{λ^2}b_x^2
\] (15)

These eigenvalues have an interesting feature: at the degeneracy point \( κ = 0 \), in the center of circuit \( C \), \( μ = 0 \) and Kramers degeneracy is not lifted, provided \( b \) is perpendicular to \( ξ \). The states at \( k^2 \) have anisotropic \( g \) factors which vanish in two directions. The vanishing Zeeman splitting means that a conical intersection, hidden unless \( b \neq 0 \), exists exactly where the original band intersection (for \( ξ = 0 \) was located. This also yields a simple geometrical phase of \( ±π \). Bands for \( b || ξ \) and \( b \perp ξ \) are shown in Fig[1] panels (b) and (c).

A full calculation of \( γ(C) \) for the 4 new eigenstates of Eq. (12) is difficult. The Berry method of solid angle works when the basis functions \( |1\rangle, |2\rangle \) of the 2 × 2 effective Hamiltonian are fixed at \( \vec{k}^* \), whereas the basis functions \( |s\rangle, |t\rangle \) or \( |u\rangle, |v\rangle \) used in Eq. (13) depend on \( \vec{k} \). However, the most important limit remaining to be resolved is when the circuit radius \( κ \) is small relative to spin-orbit splitting \( ξ \). In this limit, the basis functions lose their \( \vec{k} \)-dependence. The relevant scaled parameters are \( \vec{μ} = ((κ/λ)b_z \cos ω, -λ_z(κ/λ)b_x \sin ω, b_z) \). The circuit parameterized by \( ϕ \) is equally well parameterized by \( ω \) which evolves from 0 to 2π. The solid angle in \( \vec{μ} \)-space is 2πΛ\( λ_z (1 - b_z/μ) \), so the geometric phase is

\[
γ(C) = -πβ_3 Π \left( 1 - \frac{b_z}{\sqrt{b_z^2 + (κ/λ)^2b_x^2}} \right), \] (16)

where (\( Λ_3, β_3 \)) are the two branch indices in the eigenvalue \( ±λ ± μ = Λ_3 λ + β_3 μ \). This is the other main result of this paper. If \( b_z = 0 \), the full geometric phase \( γ(C) = ±π \) is restored no matter how small the circuit radius. Even though the degeneracy was lifted by spin-orbit interactions, the hidden conical intersection exposed by a Zeeman field controls the result.

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