Parity (and time-reversal) anomaly in a semiconductor

Oleg Tchernyshyov

School of Natural Sciences, Institute for Advanced Study, Princeton, New Jersey 08540
Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439
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Abstract

The physics of a parity anomaly, potentially observable in a narrow-gap semiconductor, is revisited. Fradkin, Dagotto, and Boyanovsky have suggested that a Hall current of anomalous parity can be induced by a Peierls distortion on a domain wall. I argue that a perturbation inducing the parity anomaly must break the time reversal symmetry, which rules out the Peierls distortion as a potential cause. I list all possible perturbations that can generate the anomaly.

I. INTRODUCTION

Condensed-matter and particle physics are cross-fertilizing fields. For instance, exclusion of magnetic flux from a superconductor was interpreted by Anderson as generation of mass for a gauge boson. Popularized in particle physics by Higgs, this effect plays a central role in the electroweak theory. In the other direction, statistical (Chern-Simons) gauge fields, a field-theorist’s toy, facilitate better understanding of the quantum Hall effect. A closely related phenomenon, parity anomaly in (2 + 1)-dimensional electrodynamics, still awaits its experimental discovery in condensed matter.

In a nutshell, the effect is rather simple. Two-component Dirac fermions with a mass $m$ react in a peculiar way to an external magnetic field $B$. The symmetry between occupied (Fermi-sea) and empty fermion states is violated and a nonzero fermion density appears in the vacuum state. The density of fermions—each carrying charge $\pm e/2$—is such that the average flux per particle is $hc/e$:

$$\rho = \frac{Q}{A} = \frac{m}{|m|} \frac{e^2 B}{2hc}. \tag{1}$$

By relativistic invariance, application of an electric field in the plane induces a Hall current with quantized conductivity:

$$J_i = (\sigma/c)\epsilon_{ij}E_j, \quad \sigma = -\frac{m}{|m|} \frac{e^2}{2\hbar}. \tag{2}$$
Both the induction of charge by magnetic field (1) and the appearance of a Chern-Simons current (2) violate the symmetries of parity and time reversal, hence the name “parity anomaly”. In certain materials, electrons behave as Dirac fermions, albeit with a small “speed of light”, so it seems natural to look for the anomaly in condensed matter.

On a deeper level, there is a subtle problem, known as fermion doubling, which often prevents the anomaly. For example, electron states in a sheet of graphite are well described at low energies as 2-component massless Dirac fermions in 2+1 dimensions. Because the unit cell contains 2 lattice sites, there are 2 fermion species living at inequivalent Fermi points in the Brillouin zone. Semenoff observed that a symmetry breaking mass term \( m \) will be induced if the inequivalent sites are populated by different atoms. Unfortunately, the 2 species have mass terms of opposite signs. The total anomalous current (2) vanishes.

Later, Fradkin, Dagotto and Boyanovsky (FDB) suggested a possible way to circumvent the problem of fermion doubling. Lead chalcogenides PbTe, PbSe, and PbS are semiconductors with a narrow gap (0.15–0.3 eV) between conduction and valence bands. Low-energy fermion quasiparticles are concentrated around 4 inequivalent L points in the Brillouin zone, \( \pm(\pi/a)(1,1,1) \) and three others related by cubic symmetry. The band structure near each L point is such that the quasiparticles resemble 4-component massive Dirac fermions (in 3+1 dimensions). 4 components result from 2 inequivalent sites in a unit cell and 2 possible projections of a spin 1/2. FDB pointed out that a stack fault in a crystal creates a domain wall, on which one finds 2+1 dimensional massless Dirac fermions. In this setting, certain perturbations can induce a mass term of the same sign in all 4 fermion species. The anomalous current (2) does not have to vanish.

In a more detailed paper, FDB suggested that a symmetry-breaking mass term \( m \) can be induced by a Peierls distortion, which is present in some lead chalcogenides. That does not sound right: a Peierls distortion violates parity but leaves time reversal intact, therefore it cannot possibly induce a Chern-Simons current (2). Haldane has argued that this incarnation of parity anomaly is caused by an unphysical lattice Hamiltonian used by FDB, which is (or seems to be) odd under time reversal. Upon further reflection, this argument does not work: if a continuum limit derives from a model with lattice potential and spin-orbit interaction, it cannot violate the time-reversal symmetry. Then why does the FDB Hamiltonian couple spin and linear momentum via the term \( \vec{\sigma} \cdot \vec{k} \) — that seems to break \( T \)? The answer: the \( \sigma \) matrices here are not the electron spin variables. Symmetry under time reversal need not be broken. The existence of the anomalous Chern-Simons current is then questionable.

Being field theorists, FDB didn’t bother to derive their Hamiltonian (nor its continuum version) from any physical model of electrons in a lattice potential and with the spin-orbit interaction. Their phenomenological Hamiltonian was merely tailored to correctly reproduce the energy spectrum of the conduction and valence bands near the Fermi level. Therefore the \( \sigma \) matrices in it have nothing to do with the actual electron spin. But without knowing which physical variables the \( \sigma \) matrices represent, one cannot learn how this or that physical perturbation (e.g., a Peierls distortion) couples to the fermion zero modes. Then it is impossible to determine correctly the sign of charge—or the direction of Hall current—induced by a symmetry-breaking perturbation.

To clear up the matter, I have derived a correct continuum approximation for low-lying electron states both by appealing to symmetry arguments (the easy way) and by using the standard \( k \cdot p \) method combined with a tight-binding approximation (see Appendix). I
have studied the behavior of massless fermions bound to a domain wall and enumerated all symmetry-breaking perturbations that raise or lower the zero modes in magnetic field, thus inducing surface charge (4). The results of this study are unambiguous. Already from Eq. it is clear that \( m \) should be odd under both parity and time reversal (a pseudoscalar). A Peierls distortion therefore will not work because \( m = q \cdot \hat{n} \) is a genuine scalar (\( q \) is the vector of atomic displacement and \( \hat{n} \) is the normal to the domain wall). On the other hand, certain kinds of magnetic order may induce an anomalous Hall current.

### II. LOW-ENERGY HAMILTONIAN

The FDB Hamiltonian (in the continuum limit) can be derived from a tight-binding model of noninteracting electrons that includes electron kinetic energy, periodic lattice potential, and spin-orbit interaction:

\[
H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) + \frac{[\hat{\sigma} \times \nabla V(\mathbf{r})] \cdot \mathbf{P}}{4m^2c^2}. \tag{3}
\]

This Hamiltonian is invariant under parity and time reversal.

The triplet of Pauli matrices \( \hat{\sigma} \) denotes the spin operators. Introduce operators of isospin \( \tau_1, \tau_2, \tau_3 \) to describe the two sublattices in the rocksalt structure. Eigenvalues \( \tau_3 = \pm 1 \) correspond to lead and chalcogen sites. Near each of the four L points, lowest-energy states have a 4-component wavefunction (2 spin components \( \times \) 2 sublattices) and resemble Dirac fermions. By symmetry arguments alone, one can anticipate the correct form of the Hamiltonian in the continuum limit.

Define the operations of parity and time reversal as

\[
P\psi(\mathbf{r}) = -\psi(-\mathbf{r}), \quad T\psi(\mathbf{r}) = \sigma_y \psi^*(\mathbf{r}). \tag{4}
\]

The minus sign accounts for odd parity of \( p \) orbitals. Near an L point in the Brillouin zone, e.g., \( \mathbf{p} = (\pi/a)(1,1,1) \), the one-particle Hamiltonian of a Dirac fermion is limited to the following \( P \) and \( T \)-invariant terms:

\[
H = -iv\tau_1(\hat{\mathbf{p}} \cdot \nabla) - iv\lambda\tau_2([\hat{\sigma} \times \hat{\mathbf{p}}] \cdot \nabla) + \tau_3 M v^2. \tag{5}
\]

Here \( \hat{\mathbf{p}} = \mathbf{p}/p \) is odd under both parity and time reversal (directions \( \hat{\mathbf{p}} \) and \( -\hat{\mathbf{p}} \) describe the same L point); \( \lambda \) is the relative strength of the spin-orbit interaction, and \( v \) is a fermion velocity. For simplicity, I set \( \lambda = 1 \), which gives a spherically symmetric energy spectrum near the L points. The same form of \( H \) is obtained from a tight-binding model, see Appendix A. The low-energy Hamiltonian thus has a Dirac form \( H = -i\hat{\alpha} \cdot \nabla + \beta M \). The standard Dirac matrices have the following representation:

\[
\hat{\alpha} = \tau_1 \hat{\mathbf{p}} + \tau_2 [\hat{\sigma} \times \hat{\mathbf{p}}], \quad \beta = \gamma^0 = \tau_3,
\]

\[
-i\gamma^1 = -i\beta\hat{\alpha} = \tau_2 \hat{\mathbf{p}} - \tau_1 [\hat{\sigma} \times \hat{\mathbf{p}}], \quad \gamma^5 = -\tau_1 (\hat{\sigma} \cdot \hat{\mathbf{p}}),
\]

\[
\Sigma = -\gamma^5 \hat{\alpha} = (\hat{\sigma} \cdot \hat{\mathbf{p}}) \hat{\mathbf{p}} + \tau_3 \hat{\mathbf{p}} \times [\hat{\sigma} \times \hat{\mathbf{p}}], \quad i\gamma^0 \gamma^5 = \tau_2 (\hat{\sigma} \cdot \hat{\mathbf{p}}). \tag{6}
\]
III. MASSLESS FERMIONS ON A DOMAIN WALL

Consider a stack fault (Pb ↔ Te) in a plane perpendicular to a unit vector $\hat{n}$. Then $M$ is a function of $x_\parallel = r \cdot \hat{n}$. More specifically, the normal to the domain wall $\hat{n}$ points in the direction of increasing $M$:

$$M(x_\parallel) \to \pm |M_0| \quad \text{for} \quad x_\parallel \equiv r \cdot \hat{n} \to \pm \infty,$$

Energy eigenstates bound to the domain wall can be written in the form $\psi(r) = u(x_\parallel)\psi(x_\perp)$, where $x_\perp = \hat{n} \times [r \times \hat{n}]$ are coordinates within the plane. The scalar $u(x_\parallel)$ and bispinor $\psi(x_\perp)$ satisfy the following equations:

$$u'(x_\parallel) = -M(x_\parallel)u(x_\parallel),$$

$$(-i\gamma \cdot \hat{n}) \psi(x_\perp) = \psi(x_\perp),$$

$$-iv \vec{\alpha} \cdot \nabla_\perp \psi(x_\perp) = E \psi(x_\perp).$$

The first two equations (8–9) indicate that these states are fermion zero modes in the direction perpendicular to the wall. The last two (9-10) describe 2-component massless fermions in 2+1 dimensions with the Hamiltonian

$$H = v \vec{\alpha} \cdot (-i \nabla_\perp - \frac{e}{c} A_\perp).$$

Application of magnetic field $B_x = B\hat{n}$ perpendicular to the domain wall results in a spectrum with Landau levels:

$$H^2 = v^2 \left(-i \nabla_\perp - \frac{e}{c} A_\perp \right)^2 - \frac{eBv^2}{c} \vec{\Sigma} \cdot \hat{n}.$$ 

The energy spectrum is symmetric with respect to charge conjugation:

$$E = 0, \pm v(2|eB|/c)^{1/2}, \pm v(4|eB|/c)^{1/2} \ldots$$

Zero modes ($E = 0$) are eigenstates of the “spin” component $\vec{\Sigma} \cdot \hat{n}$ with the eigenvalue $\text{sgn}(eB)$. All Landau levels have orbital degeneracy $|eB|/2\pi c$ per unit area.

In a half-filled system (no dopants), the zero modes are exactly at the Fermi level and thus have occupation numbers $1/2$. The energy spectrum is particle-hole symmetric and the domain wall is not charged. An arbitrarily small perturbation can shift the zero modes above or below the chemical potential (assuming it stays pinned at 0). With the particle-hole symmetry broken, the domain wall gets charged: each zero mode contributes charge $+e/2$ (empty) or $-e/2$ (filled) to the domain wall ($e < 0$).

Although a condensed-matter system lacks the true relativistic invariance and quantization of Hall conductivity does not follow automatically from Eq. 4, there is a thermodynamic identity that establishes this relation:

$$\sigma = -\left. \frac{\partial \rho}{\partial B} \right|_{\mu=\text{const}} = -\frac{m}{|m|} \frac{e^2}{2\hbar},$$

with the derivative taken at a constant chemical potential. This result is valid in the absence of low-energy excitations.
IV. SYMMETRY-BREAKING PERTURBATIONS

Imagine now that a uniform perturbation $V$ (such as a Peierls distortion or the actual Zeeman term) is applied to fermions on the domain wall. In the presence of the Landau gap, the shift of the zero modes can be computed to first order in $V$ using the standard perturbation theory. Because there is no spin or isospin degeneracy and $V$ is uniform, $\Delta E = \int \psi^\dagger V \psi \, d^3r$.

Recall that $\psi$ is an eigenstate of 3 commuting matrices:

\begin{align*}
(\vec{\Sigma} \cdot \hat{n}) \psi &= \text{sgn}(eB) \psi, \\
(-i\vec{\gamma} \cdot \hat{n}) \psi &= \psi, \\
(i\gamma^0\gamma^5) \psi &= \text{sgn}(eB) \psi.
\end{align*}

(The third matrix $\gamma^0\gamma^5$ is simply the product of the first two.) To compute $\psi^\dagger V \psi$, one can write $V$ as a superposition of 15 traceless Hermitian $4 \times 4$ matrices 

\begin{align*}
\{H_i\} &= \{\gamma^0, \gamma^5, i\gamma^0\gamma^5, \vec{\alpha}, -i\vec{\gamma}, \vec{\Sigma}, \gamma^0\vec{\Sigma}\}:
\end{align*}

$$
\psi^\dagger V \psi = \sum_{i=1}^{15} \frac{1}{4} \text{Tr}(VH_i) \psi^\dagger H_i \psi
$$

Because operators $H_i$ either commute or anticommute with one another, only 3 of them (15–17) need to be included in the sum: if some $H_j$ anticommutes with one of them, its expectation value in the state $\psi$ vanishes.

Thus operators (15–17) exhaust all the handles through which external perturbations can tickle the zero modes and possibly induce charge on a domain wall. Such a perturbation will contain $F_\Sigma \vec{\Sigma} \cdot \hat{n}$, $-iF_\gamma \vec{\gamma} \cdot \hat{n}$, or $iF_5 \gamma^0\gamma^5$. The symmetry breaking term $F_\Sigma$ is a pseudovector, $F_\gamma$ is a vector, and $F_5$ is a pseudoscalar. The area density of charge induced by them on a domain wall (for a single fermion species) is

$$
-\text{sgn}(F_\Sigma \cdot \hat{n}) \frac{e^2(B \cdot \hat{n})}{4\pi c h},
-\text{sgn}(F_\gamma \cdot \hat{n}) \frac{e|eB|}{4\pi c h},
-\text{sgn}(F_5) \frac{e^2(B \cdot \hat{n})}{4\pi c h}.
$$

It is now evident that a vector perturbation $F_\gamma$, such as a Peierls distortion, cannot induce a Chern-Simons current: the sign of induced charge is not sensitive to the direction of magnetic field. By the thermodynamic identity (14), there will be a normal Hall effect with current reversing the direction when magnetic field does.

One obviously needs a pseudoscalar perturbation (odd under both $P$ and $T$) in order to relate a scalar (charge) to the pseudoscalar $B \cdot \hat{n}$. This is why a pseudoscalar $F_5$ will work (and a vector $F_\gamma$ will not). Alternatively, one can use a pseudovector $F_\Sigma$ (e.g., staggered field of an antiferromagnetic order parameter) to construct a pseudoscalar $(F_\Sigma \cdot \hat{n})$.

To corroborate these general considerations, I discuss in some detail several symmetry-breaking terms that might exist in a physical system.
A. Peierls distortion

We need to add to the 3 + 1 dimensional Dirac Hamiltonian (3) a term that breaks $P$ but not $T$ and does not affect electron spin. Such a term is

$$V = \tau_2 (\mathbf{q} \cdot \mathbf{p})$$

(both $\tau_2$ and $\mathbf{p}$ are $T$-odd). The vector $\mathbf{q}$ characterizes the direction and length of the Peierls distortion. It couples to the operator $-i\mathbf{\gamma} \cdot \mathbf{n}$ (16). With the aid of Eq. 18,

$$\Delta E = \frac{1}{4} \text{Tr} \left( \tau_2 (\mathbf{q} \cdot \mathbf{p}) (-i\mathbf{\gamma} \cdot \mathbf{n}) \right) = (\mathbf{q} \cdot \mathbf{p}) (\mathbf{p} \cdot \mathbf{n}).$$

(21)

The charge density is unchanged when magnetic field is reversed $B \rightarrow -B$. By extension (14), the Hall conductivity is sensitive to the direction of $B$. For a wall perpendicular to $\mathbf{q}$, summation over the four L points gives

$$\sigma = \frac{2e^2}{h} \text{sgn}(eB).$$

(22)

This describes a perfectly normal Hall current, not a Chern-Simons current (2). No parity anomaly here.

B. Zeeman effect: uniform magnetic field

Consider Zeeman interaction $V = -ge(\mathbf{B} \cdot \mathbf{\sigma})/2mc$ induced by uniform magnetic field $\mathbf{B}$ perpendicular to the domain wall.

$$\Delta E = -\frac{ge}{2mc} \frac{1}{4} \text{Tr} \left( (\mathbf{B} \cdot \mathbf{\sigma}) (\mathbf{\Sigma} \cdot \mathbf{n}) \right) \text{sgn}(eB) = -\frac{g|eB|}{2mc} (\mathbf{p} \cdot \mathbf{n})^2.$$

(23)

At a constant chemical potential,

$$Q = \frac{4e|eB|}{4\pi c} \text{sgn}(g).$$

(24)

Again, a normal Hall effect results:

$$\sigma = -\frac{2e^2}{h} \text{sgn}(geB).$$

(25)

C. Zeeman effect: staggered magnetic field

In a system with antiferromagnetic order, one expects staggered magnetic field $\mathbf{B}_{st}$ to induce a Zeeman term $V = -\tau_3 g e (\mathbf{B}_{st} \cdot \mathbf{\sigma})/2mc$. It couples to the same operator of Dirac “spin” (13):

$$\Delta E = -\frac{ge}{2mc} \frac{1}{4} \text{Tr} \left( \tau_3 (\mathbf{B}_{st} \cdot \mathbf{\sigma}) (\mathbf{\Sigma} \cdot \mathbf{n}) \right) \text{sgn}(eB) = -\frac{g|e|\text{sgn}(B)}{2mc} ([\mathbf{p} \times [\mathbf{B}_{st} \times \mathbf{p}] \cdot \mathbf{n}).$$

(26)
In the simple case with $B_{st} = B_{st} \hat{n}$,

$$\frac{Q}{A} = \frac{4e^2 B}{4\pi c} \text{sgn}(geB_{st}) \quad (27)$$

and

$$\sigma = -\frac{2e^2}{h} \text{sgn}(geB_{st}). \quad (28)$$

The Hall current depends on the direction of the staggered field $B_{st}$ and not of the uniform field $B$. One can call this a parity anomaly, but clearly there is no magic involved: this is a Hall effect caused by the staggered magnetic field.

**D. A pseudoscalar?**

Finally, one can imagine coupling directly to the third conserved quantity $Q$. The only perturbation that will do is

$$V = \delta \tau_2 (\vec{\sigma} \cdot \vec{p}). \quad (29)$$

The sign of induced charge depends on the direction of magnetic field:

$$\frac{Q}{A} = \frac{-4e^2 B}{4\pi c} \text{sgn}(\delta). \quad (30)$$

Hall conductivity is insensitive to the sign of $B$:

$$\sigma = \frac{2e^2}{h} \text{sgn}(\delta). \quad (31)$$

This term definitely generates a Chern-Simons current. I must admit though that I do not understand what perturbation could cause it.

**V. CONCLUDING REMARKS**

I have presented a critique of the parity anomaly (Eqs. 1 and 2) suggested for $2+1$ dimensional fermions in a narrow-gap semiconductor. Both symmetry considerations and a correct continuum treatment of the model indicate that a parity anomaly requires a pseudoscalar ($P$ and $T$-odd) or pseudovector ($P$-even and $T$-odd) symmetry-breaking term. Therefore, a Peierls distortion, which is a vector ($P$-odd and $T$-even), cannot generate a parity anomaly, contrary to the suggestion of FDB.

Antiferromagnetic order, which violates the time-reversal symmetry, could lead to an observable Chern-Simons current in the system. Unfortunately, the prospects of observing such an effect are rather dim: not only would this require antiferromagnetism, but also the Néel order parameter must be (anti)parallel to the applied magnetic field. In a Heisenberg antiferromagnet, $B_{st}$ stays orthogonal to $B$, in which case the entire effect vanishes.

In hindsight, this foray into the dreamworld of field theory is a reminder to a condensed-matter physicist: trust your intuition. Anomalous Hall current of Dirac fermions, whether directly in $d = 2 + 1$ dimensions or on a domain wall in $d = 3 + 1$, is always caused by magnetic order present in the system.
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APPENDIX A: DIRAC FERMIONS FROM A TIGHT-BINDING MODEL

Lead and a chalcogen have 2 and 4 electrons in their 3 external \( p \) orbitals (\( s \) orbitals give deeply lying bands, which can be ignored). The \( p \) bands are thus half filled. The one-particle Hamiltonian including lattice potential and spin-orbit interaction is

\[
H = - \frac{\nabla^2}{2m} + V(r) + \frac{[\vec{\sigma} \times \nabla V(r)] \cdot (-i \nabla)}{4m^2c^2}.
\]

(A1)

Omitting spin for clarity, one can write an energy eigenfunction in the Bloch form

\[
\Psi_p(R) = \sum_i \sum_\alpha \psi^{\alpha i}(R - r - \Delta r^{\alpha}) \phi^{\alpha i}_p(r) e^{ip \cdot (r + \Delta r^{\alpha})}.
\]

(A2)

Here \( r \) labels unit cells in the rocksalt lattice, \( \Delta r^{\alpha} \) are the coordinates of site \( \alpha \) within a unit cell and \( \psi^{\alpha i}(R) \) is the wavefunction of the \( i \)-th orbital on sublattice \( \alpha \). We are to find the Bloch coefficients \( \phi^{\alpha i}_p(r) \). With spin included, \( \phi^{\alpha i\sigma}_p(r) \) is a 12-component wave function.

It follows from symmetry considerations alone \( \square \) that the two sublattices (lead and chalcogen sites) are decoupled at the L points, such as \( \mathbf{p} = \pm (\pi/a)(1, 1, 1) \). In this case, the Hamiltonian takes on a simple form \( \square \)

\[
H_\alpha = 2W_\alpha \cos \left( \frac{2}{3} \mathbf{L} \cdot \mathbf{\hat{p}} \right) + \lambda_\alpha \mathbf{\hat{L}} \cdot \mathbf{\hat{L}},
\]

(A3)

where the first term comes from the overlap of different \( p \) orbitals (between second neighbors) and the second, from the spin-orbit interaction. The eigenstates of the Hamiltonian (A3) are Kramers doublets with \( \mathbf{J} \cdot \mathbf{\hat{p}} = \pm 1/2 \) or \( \pm 3/2 \). According to Volkov \( \textit{et al.} \square \) the spin-orbit coupling is the weakest perturbation and the two bands around the Fermi level are derived from states with \( \mathbf{L} \cdot \mathbf{\hat{p}} = 0 \). In this approximation, \( \square \) the eigenstates are

\[
\phi^{\alpha \sigma}_p(r) = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \otimes |\sigma_z = \sigma\rangle,
\]

(A4)

in the basis of \( p_x, p_y, p_z \) orbitals.

To calculate the matrix elements of the Hamiltonian near an L point, at lattice momentum \( \mathbf{p} + \mathbf{k} \), I use the standard “\( \mathbf{k} \cdot \mathbf{p} \)” method \( \square \). Instead of shifting momentum away from a symmetry point \( \mathbf{p} \rightarrow \mathbf{p} + \mathbf{k} \) in the wavefunctions (A2), one transforms the Hamiltonian

\[
H \rightarrow e^{-i\mathbf{k} \cdot \mathbf{R}} H e^{i\mathbf{k} \cdot \mathbf{R}} = H + \frac{1}{m} \mathbf{k} \cdot \left( -i \nabla + \frac{\vec{\sigma} \times \nabla V(R)}{4mc^2} \right).
\]

(A5)
The matrix elements of the second term “(k·p)/m” are then evaluated in the Hilbert space of the two Kramers doublets closest to the Fermi level at the L point. This is a good approximation for small k, provided that other states lie at energies much larger than the gap Δ = (Ep - Et)/2.

In the tight-binding limit, overlap of px orbitals on different sublattices occurs along the x direction only. In the case of px orbitals at momentum px = π/a (Fig. 1), operators −i∇ and ∇V(R) have the following nonzero matrix elements:

\[ \langle Pb, x = 0|(-i\partial_x)|Te, x = a/2\rangle = C_1, \quad (A6) \]
\[ \langle Pb, x = 0|\partial_x V|Te, x = a/2\rangle = iC_2, \quad (A7) \]

where C_1 and C_2 are some real constants. In the basis of states px, py, pz, the resulting k·p term reads

\[ C_1\tau_1 \begin{pmatrix} k_x & 0 & 0 \\ 0 & k_y & 0 \\ 0 & 0 & k_z \end{pmatrix} + C_2\tau_2 \begin{pmatrix} k_y\sigma_z - k_z\sigma_y & 0 & 0 \\ 0 & k_z\sigma_x - k_x\sigma_z & 0 \\ 0 & 0 & k_x\sigma_y - k_y\sigma_x \end{pmatrix} \quad (A8) \]

near the L point p = (π/a)(1, 1, 1). The operators of isospin \( \tau \) act according to

\[ \tau_1|Pb\rangle = |Te\rangle, \ \tau_2|Pb\rangle = i|Te\rangle, \ \tau_3|Pb\rangle = |Pb\rangle, \ \tau_3|Te\rangle = -|Te\rangle. \quad (A9) \]

Matrix elements of the complete Hamiltonian between the states (A4) are:

\[ \frac{1}{3}C_1\tau_1 (k_x + k_y + k_z) + \frac{1}{3}C_2\tau_2 [(k_y - k_z)\sigma_x + (k_z - k_x)\sigma_y + (k_x - k_y)\sigma_z] + \frac{1}{2}(Ep - Et)\tau_3. \quad (A10) \]

This yields the anticipated continuum result (5)

\[ H = v(k\cdot\hat{p})\tau_1 + \lambda v(k\cdot[\hat{p}\times\vec{\sigma}])\tau_2 + Mu^2\tau_3, \quad (A11) \]

where \( \hat{p} \) is the unit vector in the direction of the L point p = (π/a)(1, 1, 1). An identical result is obtained for the 3 other L points, which differ by the direction \( \hat{p} \).

On a final note, the unit vector \( \hat{p} = p/p \) is odd under parity and time reversal defined in Eq. 4. It can be made even by redefining them as

\[ P\psi(r) = -\tau_3\psi(-r), \ T\psi(r) = \tau_3\sigma_y\psi^*(r). \quad (A12) \]

This is the familiar standard representation of parity and time reversal in relativistic field theory.\[2\]
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FIG. 1. Calculation of overlap integrals for adjacent $p_x$ orbitals. Momentum $p_x = \pi/a$. 

![Diagram showing overlap integrals for adjacent $p_x$ orbitals with labels for Te and Pb atoms. The diagram includes symbols $+i$, $-i$, $+$, and $-i$ for the overlap integrals.](image-url)