SOME APPLICATIONS OF THE PHYSICS OF EXCEPTIONAL POINTS TO TOPOLOGICAL SEMIMETALS*

*Work in collaboration with R. A. Molina
(M. Neupane et al., Nature Commun. 5, 4786 (2014))

2014


2007

(S.-Y. Xu et al., Science 349, 613 (2015))

2015
TOPOLOGICAL SEMIMETALS

One of the most relevant properties of the topological materials is the existence of gapless excitations at their surface.

In Weyl semimetals we have the Fermi arcs connecting the projection of the Weyl nodes onto a given surface of the material.

But, in general, in the topological semimetals there is the question of the stability (topological protection) of the surface states. In the case of the Dirac semimetals, it has been claimed that surface states do not have topological protection (M. Kargarian, M. Randeria, and Y.-M. Lu, PNAS 113, 8648 (2016)).

(M. Kargarian, M. Randeria and Y.-M. Lu, PNAS 113, 8648 (2016))

TOPOLOGICAL SEMIMETALS

We are going to address the question of the stability of the surface states by focusing on their microscopic structure, in particular on their evanescence for complex values of the momentum

\[ \psi(\mathbf{r}) \sim e^{ik_z z} e^{-\alpha z} \chi \]

This will place the discussion in the context of the non-hermitian hamiltonians, which can have interesting physical applications. There has been actually a proposal to trade the hermiticity of any admissible hamiltonian $H$ by the invariance under $PT$ symmetry ($P =$ spatial inversion, $T =$ time-reversal)

\[ [H, PT] = 0 \]

In the case of an interaction potential $V$, this means that $V(\mathbf{r}) = V^*(-\mathbf{r})$. Then, the eigenvalues of $H$ can be real provided that the eigenvectors are also invariant under $PT$.

In optics, we have examples like the case of a two-channel system with gain/loss

\[
\begin{align*}
  i \frac{dE_1}{dz} &= i \frac{\gamma}{2} E_1 + \kappa E_2 \\
  i \frac{dE_2}{dz} &= \kappa E_1 - i \frac{\gamma}{2} E_2
\end{align*}
\]

The eigenvalues remain real up to $\frac{\gamma}{2 \kappa} = 1$  

(C. E. Rüter et al., Nature Phys. 6, 192 (2010))
EXCEPTIONAL POINTS IN TOPOLOGICAL SEMIMETALS

We investigate the microscopic structure of the surface states with

\[ H_W = (m_0 + m_1 \nabla^2) \sigma_x - iv(\sigma_y \partial_y + \sigma_z \partial_z) \]

This model has two bands in the bulk

\[ \varepsilon(k) = \pm \sqrt{(m_0 - m_1 k_y^2)^2 + v^2 k_y^2 + v^2 k_z^2} \quad \text{nodes at} \quad k_x = \pm \sqrt{\frac{m_0}{m_1}} \]

We can also look for surface states decaying from \( z = \text{cons.} \)

\[ \psi(r) \sim e^{i k_x x} e^{i k_z z} e^{-\alpha z} \chi \]

The eigenvalue problem is (taking for simplicity \( k_y = 0 \))

\[ (m_0 - m_1 (k_x^2 + k_z^2 - \alpha^2 + 2ik_z \alpha))\sigma_x \chi + v(k_z + i\alpha)\sigma_z \chi = \varepsilon \chi \]

Zero-energy solutions can be found for \( \chi \) such that \( \sigma_y \chi = \pm \chi \)

\[ (m_0 - m_1 (k_x^2 + k_z^2 - \alpha^2 + 2ik_z \alpha))\chi \pm iv(k_z + i\alpha) \chi = 0 \]

which leads to two different types of surface states

\[ \alpha = \frac{v}{2m_1} \]

\[ k_z = \pm \sqrt{\frac{m_0}{m_1} - \alpha^2 - k_x^2} \]

(valid only for \( 4m_0m_1 > v^2 \))

\[ \alpha = \frac{v \pm \sqrt{v^2 - 4m_1(m_0 - m_1 k_x^2)}}{2m_1} \]

\[ k_z = 0 \]

(general solution if \( 4m_0m_1 < v^2 \))

EXCEPTIONAL POINTS IN TOPOLOGICAL SEMIMETALS

\[ \alpha = \frac{\nu}{2m_1} \]

\[ k_z = \pm \sqrt{\frac{m_0}{m_1} - \alpha^2 - k_x^2} \]

(valid only for \( 4m_0m_1 > \nu^2 \))

\[ \alpha = \frac{\nu \pm \sqrt{\nu^2 - 4m_1(m_0 - m_1k_x^2)}}{2m_1} \]

\[ k_z = 0 \]

(general solution if \( 4m_0m_1 < \nu^2 \))

We can distinguish between two different types of semimetals

A type \((4m_0m_1 > \nu^2)\)

\[ \begin{align*}
0 &\leq |k_x| < \sqrt{\frac{m_0}{m_1} - \frac{\nu^2}{4m_1^2}} \\
\sqrt{\frac{m_0}{m_1} - \frac{\nu^2}{4m_1^2}} &< |k_x| < \sqrt{\frac{m_0}{m_1}}
\end{align*} \]

evanescence + oscillation

pure evanescence

B type \((4m_0m_1 < \nu^2)\)

\[ 0 \leq |k_x| < \sqrt{\frac{m_0}{m_1}} \]

pure evanescence
EXCEPTIONAL POINTS IN TOPOLOGICAL SEMIMETALS

\[ \Delta \text{ type } \quad (4m_0m_1 > v^2) \]

\[ 0 \leq |k_x| < \sqrt{\frac{m_0}{m_1} - \frac{v^2}{4m_i^2}} \]

evanescence + oscillation

\[ \sqrt{\frac{m_0}{m_1} - \frac{v^2}{4m_i^2}} < |k_x| < \sqrt{\frac{m_0}{m_1}} \]

pure evanescence

\[ \text{B type } \quad (4m_0m_1 < v^2) \]

\[ 0 \leq |k_x| < \sqrt{\frac{m_0}{m_1}} \]

pure evanescence

The two different types of surface states have quite distinct behavior, which becomes more apparent in a slab geometry (with nonnegligible coupling between opposite faces).
EXCEPTIONAL POINTS IN TOPOLOGICAL SEMIMETALS

A closer look reveals that the evanescent states correspond to branch points (square-root singularities) in the spectrum for complex momentum $k_z + i\alpha$

$$k_x = 0$$

A type

$$k_x = 0$$

B type

The branch points are so-called exceptional points in the spectrum of the non-hermitian hamiltonian, which endow the surfaces states with topological protection

The existence of two branch cuts can be understood from the symmetries of the hamiltonian

$$P: \psi(r) \longrightarrow \sigma_x \psi(-r) \quad T: \psi(r) \longrightarrow K \sigma_x \psi(r) \quad \text{at} \quad y = \text{const}$$

EXCEPTIONAL POINTS IN TOPOLOGICAL SEMIMETALS

What we learn from the exceptional points is that the surface states are less protected in the B type semimetals, since the distance between points with opposite $\alpha$ may become very short.

In fact, the branch points with opposite $\alpha$ tend to coalesce as one approaches the endpoints of the Fermi arcs, which explains that relevant perturbations start to destroy them at the projection of the nodal points. This is consistent with the evidence provided by M. Kargarian, M. Randeria, and Y.-M. Lu, PNAS 113, 8648 (2016),
EXCEPTIONAL POINTS

Exceptional points are well-known in the study of non-hermitian hamiltonians

\[ H(\lambda) = H_0 + \lambda V = \begin{pmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{pmatrix} + \lambda \begin{pmatrix} \epsilon_1 & \delta_1 \\ \delta_2 & \epsilon_2 \end{pmatrix}. \]

But they have been mainly discussed in optics. In the system of two coupled waveguides with gain and loss

\[ i \frac{dE_1}{dz} = i \frac{\gamma}{2} E_1 + \kappa E_2, \]
\[ i \frac{dE_2}{dz} = \kappa E_1 - i \frac{\gamma}{2} E_2. \]

There is a phase transition at \( \frac{\gamma}{2\kappa} = 1 \)

The eigenvectors are

\[ |\pm\rangle = \begin{pmatrix} 1 \\ \pm e^{\pm i\theta} \end{pmatrix} \quad \frac{\gamma}{2\kappa} < 1, \quad |\pm\rangle = \begin{pmatrix} 1 \\ i e^{\pm \delta} \end{pmatrix} \quad \frac{\gamma}{2\kappa} > 1 \]

(from C. E. Rüter et al., Nature Phys. 6, 192 (2010))
EXCEPTIONAL POINTS IN TOPOLOGICAL SEMIMETALS

Recently, some applications have started to be found in electron systems:

- V. Kozii and L. Fu, Non-Hermitian Topological Theory of Finite-Lifetime Quasiparticles: Prediction of Bulk Fermi Arc Due to Exceptional Point, arXiv:1708.05841
Interesting physics arises in topological semimetals in strong magnetic fields:

- closed orbits connecting Fermi arcs in Weyl semimetals (A. C. Potter, I. Kimchi and A. Vishwanath, Nat. Commun. 5, 5161 (2014))

EXCEPTIONAL POINTS IN TOPOLOGICAL SEMIMETALS

The same description applies to nodal-line semimetals

\[ H_{NL} = (m_0 + m_1 \nabla^2) \sigma_x - iv \sigma_z \partial_z \]

This model leads to a spectrum in the bulk

\[ \varepsilon(k) = \pm \sqrt{(m_0 - m_1 k_x^2)^2 + v^2 k_z^2} \]

with a ring of nodes at \( k_z = 0 \) for \( k_x^2 + k_y^2 = \frac{m_0}{m_1} \)

There are also surface states which can be obtained as evanescent waves decaying from \( z = \text{const} \)

\[ \psi(r) \sim e^{ik_z z} e^{-\alpha z} \chi \]

The evanescent waves correspond to exceptional points in the extension of the spectrum to complex momentum, surviving under very general perturbations

(W. B. Rui, Y. X. Zhao, and A. P. Schnyder, arXiv:1703.05958)
NODAL-LINE SEMIMETALS IN STRONG MAGNETIC FIELDS

For a uniform magnetic field perpendicular to the nodal ring

\[ H_{NL} = (m_0 + m_1 \nabla^2) \sigma_x - i v \sigma_z \partial_z \]
\[ \Downarrow \quad A = (-B y, 0, 0) \]

\[ H_\perp = \left( m_0 + m_1 \left( -\left( k_x - B y \right)^2 + \partial_y^2 + \partial_z^2 \right) \right) \sigma_x - i v \sigma_z \partial_z \]

In the bulk we have energy levels (with degeneracy label by \( k_x \))

\[ \varepsilon_n(k) = \pm \sqrt{\left( m_0 - m_1 k_z^2 - 2 m_1 B (n + 1/2) \right)^2 + v^2 k_z^2} \]

We can now look for Landau states decaying from \( z = \text{const.} \)

\[ \psi(r) \sim e^{i k_x x} e^{i k_z z} \Phi_n \left( y - \frac{k_x}{B} \right) \chi \]

The spinor \( \chi \) must satisfy

\[ \left( m_0 - m_1 \left( 2 B(n + 1/2) + k_z^2 - \alpha^2 + 2 i k_z \alpha \right) \right) \sigma_x \chi + \nu (k_z + i \alpha) \sigma_z \chi = \varepsilon \chi \]

Zero-energy solutions are found again for \( \chi \) such that \( \sigma_y \chi = \pm \chi \)

\[ \alpha = \frac{v}{2 m_1} \]

\[ k_z = \pm \sqrt{\frac{m_0}{m_1} - \alpha^2 - 2 B(n + 1/2)} \]

(valid only for \( 4 m_0 m_1 > v^2 \))

\[ \alpha = \frac{v \pm \sqrt{v^2 - 4 m_1 \left( m_0 - m_1 2 B(n + 1/2) \right)}}{2 m_1} \]

\[ k_z = 0 \]

(general solution if \( 4 m_0 m_1 < v^2 \))
NODAL-LINE SEMIMETALS IN STRONG MAGNETIC FIELDS

One can actually compute the complex spectrum from

\[
(m_0 - m_1 \left( 2B(n + 1/2) + k_z^2 - \alpha^2 + 2ik_z\alpha \right)) \sigma_x \chi + v(k_z + i\alpha)\sigma_z \chi = \varepsilon \chi
\]

It turns out that the zero-energy eigenvalues are exceptional points in the \((k_z, \alpha)\) complex plane. This means that the Landau surface states share the topological protection of the drumhead surface states.

The Landau surface states do not carry in general electronic current since \(j_x = -2m_1(k_x - By)\sigma_x\) while the surface states are practically eigenstates of \(\sigma_y\) in slabs with little coupling between opposite faces. This does not hold however when approaching the boundaries of the lateral dimension \(y\). In that case

\[
\frac{\partial \varepsilon}{\partial k_x} \neq 0 \quad \Rightarrow \quad \langle j_x \rangle \neq 0
\]

For a uniform magnetic field parallel to the nodal plane

\[ H_{\text{NL}} = (m_0 + m_1 \nabla^2) \sigma_x - i \nu \sigma_z \partial_z \]

\[ \downarrow \quad A = (Bz, 0, 0) \]

\[ H_{\|} = \left( m_0 + m_1 \left( -k_x^2 - k_y^2 + \partial_z^2 \right) \right) \sigma_x - i \nu \sigma_z \partial_z \]

The model cannot be solved exactly, but numerical resolution shows the existence of zero-energy states in the bulk localized in 2D slices with \( z = \text{const.} \).

At \( k_x = k_y = 0 \),

\[ \left( m_0 + m_1 \left( \partial_z^2 - B^2 z^2 \right) \right) \sigma_x \chi - i \nu \sigma_z \chi = \varepsilon \chi \]

looks like an equation for massive Dirac fermions, with two domain walls (turning points) which pin a pair of evanescent waves and lead to the appearance of midgap states.
The quasi-2D states can be shifted in the bulk by varying $k_x$, leading to dispersing bands when the slice approaches one of the faces of the slab. In general, there is a huge degeneracy of the zero Landau level, from the collapse of a number of flat bands with different $k_y$.

The current across the whole section of the slab (for each state) is

$$\langle j_x \rangle = \frac{\partial \epsilon}{\partial k_x}$$

which implies

$$I_x = \frac{e}{\hbar} \int_{\text{filled states}} \frac{dk_x}{2\pi} \frac{\partial \epsilon}{\partial k_x}$$

This leads to a quantization condition $\sigma_{xz} = Ne^2/h$, with values of $N$ which scale linearly with $\Delta y$.

WEYL SEMIMETALS UNDER CIRCULARLY POLARIZED LIGHT

We start with a model of Weyl semimetal

\[ H_0 = M(\mathbf{k}) \sigma_z + v k_x \sigma_x + v k_y \sigma_y \]
\[ M(\mathbf{k}) = m_0 - m_1 k_z^2 - m_2 (k_x^2 + k_y^2) \]

We shine light in the direction along the line of the nodes

\[ \mathbf{k} \rightarrow \mathbf{k} + A(\cos(\Omega t), \sin(\Omega t), 0) \]

We use Floquet theory to find the solutions of the time-dependent Schrödinger equation

\[ -i \partial_t |\Psi(t)\rangle = H(t) |\Psi(t)\rangle \]
\[ |\Psi'(t)\rangle = e^{-i\varepsilon t} |\Phi(t)\rangle \quad , \quad |\Phi(t+T)\rangle = |\Phi(t)\rangle \quad T = \frac{2\pi}{\Omega} \]

which amounts to find the result of hybridizing a number of Floquet subbands

\[ |\Phi(t)\rangle = \sum_m e^{-im\Omega t} |\chi^{(\alpha)}_m\rangle \quad , \]
\[ \sum_n H_{mn} |\chi_n^{(\alpha)}\rangle \equiv (\varepsilon_\alpha + m\Omega) |\chi_m^{(\alpha)}\rangle \]
\[ H_{mn} = \frac{1}{T} \int_0^T dt \ H(t) \ e^{i(m-n)\Omega t} \]
Floquet topological insulators can be devised by establishing a resonance between bands with different pseudospin configuration.
WEYL SEMIMETALS UNDER CIRCULARLY POLARIZED LIGHT

The band structure is therefore periodic in energy

\[ \sum_n H_{nn} |\chi_n^{(\alpha)}\rangle = (\epsilon_\alpha + m\Omega) |\chi_m^{(\alpha)}\rangle \]

In our model we have

\[ H_{nn} = H_0 + n\Omega \mathbf{1} - m_2 A^2 \sigma_z \]
\[ H_{n+1,n} = (v/2)A(i\sigma_x - \sigma_y) + m_2 A(-ik_x - k_y)\sigma_z \]
\[ H_{n-1,n} = (v/2)A(-i\sigma_x - \sigma_y) + m_2 A(ik_x - k_y)\sigma_z \]

The hybridization of the Floquet subbands gives rise to a gap over an extended ring in momentum space:

- proportional to \( A \) (at \( \epsilon = \Omega/2 \)) between subbands \( n = 0 \) (green) and \( n = \pm 1 \) (blue/red)
- proportional to \( A^2 \) (at \( \epsilon = 0 \)) between subbands \( n = -1 \) (red) and \( n = 1 \) (blue)

\[ v = 1.1 \text{ eV \ Å} \]
\[ \Omega = 0.5 \text{ eV} \]
\[ A = 0.05 \text{ \ Å}^{-1} \]
WEYL SEMIMETALS UNDER CIRCULARLY POLARIZED LIGHT

But most interestingly, we can have evanescent states localized at the irradiated surface.

These states come as solutions with real quasi-energy $\varepsilon_\alpha$ for complex momenta $k_z$

$$\chi^{(\alpha)} \sim e^{i k_z z} , \quad k_z = k_R + i k_I$$

Computing for a wire with finite section in the $x$-$y$ plane (150 $\times$ 150 $\text{Å}^2$)

![Graph showing band structure and evanescent states](image)

we find evanescent states (for $\text{Im}(k_z) \approx 0.01$ $\text{Å}^{-1}$) at the position of the dots within the gap between Floquet subbands in the figure.

WEYL SEMIMETALS UNDER CIRCULARLY POLARIZED LIGHT

We can have a deeper insight by solving for a single Weyl cone

\[ H_W = -iv\sigma_x \hat{\partial}_x - iv\sigma_y \hat{\partial}_y - iv_z \sigma_z \hat{\partial}_z \]
\[ + \nu A(\sigma_x \cos(\Omega t) + \sigma_y \sin(\Omega t)) \]

\(H_W\) can be translated to time-independent form by making a unitary transformation

\[ \tilde{H}_W = U^+ H_W U - iU^+ \partial_t U \]
\[ = -iv\sigma_x \hat{\partial}_x - iv\sigma_y \hat{\partial}_y - iv_z \sigma_z \hat{\partial}_z - \Omega J_z + \nu A \sigma_x \]
\[ J_z = -i\hat{\partial}_\theta + \sigma_z / 2 \]

and transforming again we obtain

\[ \tilde{H}_W' = P^+ \tilde{H}_W P \]
\[ = -iv\sigma_x \hat{\partial}_x - iv\sigma_y \hat{\partial}_y - iv_z \sigma_z \hat{\partial}_z \]
\[ - \Omega J_z - \Omega Ar \sin(\theta) \]
\[ J_z = -i\hat{\partial}_\theta + \sigma_z / 2 \]

We find that the spectrum has a gap between Floquet subbands with \( j_z = 1/2 \) and \( j_z = -1/2 \)

\[ \nu = 1.1 \text{ eV Å} \]
\[ \Omega = 0.5 \text{ eV} \]
\[ A = 0.005 \text{ Å}^{-1} \]
WEYL SEMIMETALS UNDER CIRCULARLY POLARIZED LIGHT

The gap has oscillations as a function of $k_z$ which have a correspondence with points with zero eigenvalue in the complex plane.

$v = 1.1 \text{ eV } \text{Å}$
$\Omega = 0.5 \text{ eV}$
$A = 0.005 \text{ Å}^{-1}$
$\text{Im}(k_z) = 0.08 \text{ Å}^{-1}$

The form of $\text{Im}(\varepsilon)$ is indeed the signature of a behavior of the form

$$\varepsilon(k_z) \sim \sqrt{p_n - k_z} \sqrt{p_n - k_z}$$

The set of exceptional points corresponds to a sequence of zero-energy evanescent states, with a peculiar quantization pattern.

$$\text{Re}(p_1) > \text{Re}(p_2) > \text{Re}(p_3) \ldots$$

WEYL SEMIMETALS UNDER CIRCULARLY POLARIZED LIGHT

The most important feature of the evanescent states is that they carry an angular current $j_\theta$

$$j_\theta = -\frac{\sin(\theta)}{r} \nu \gamma^+ \sigma_z \psi + \frac{\cos(\theta)}{r} \nu \gamma^+ \sigma_y \psi$$

$j_\theta$ can be computed in the space spanned by the states with $j_z = \pm 1/2$

$$\chi = \begin{pmatrix} \phi_1(r) \\ e^{i\theta} \phi_2(r) \\ e^{i\theta} \phi_3(r) \\ \phi_4(r) \end{pmatrix} e^{ik_zz} + \begin{pmatrix} e^{-i\theta} \phi_1(r) \\ \phi_2(r) \\ \phi_3(r) \\ e^{-i\theta} \phi_4(r) \end{pmatrix} e^{ik_zz}$$

bearing in mind that the original states are expressed as

$$\psi = \exp(-iJ_z \Omega t) \exp(-iAr \cos(\theta)) \chi$$

The angular current has a uniform component, which is in general negligible,

$$j_{\text{static}}^\theta = -i \nu \left( \frac{1}{r} \phi_1^*(r) \phi_2(r) + \phi_3^*(r) \phi_4(r) \right) + \text{h.c.}$$

and a time-dependent component

$$j_{\Omega}^\theta = -i \nu \left( \frac{1}{r} \phi_1^*(r) \phi_4(r) e^{-i(\theta-\Omega t)} + \phi_3^*(r) \phi_2(r) e^{i(\theta-\Omega t)} \right) + \text{h.c.}$$
WEYL SEMIMETALS UNDER CIRCULARLY POLARIZED LIGHT

In a cylindrical geometry, the current has a component which rotates with frequency $\Omega$

$$j^\theta_\Omega (r, \theta; t) = \frac{v}{r} f(r, \theta - \Omega t)$$

This implies the time-dependence of the probability density of the surface states

$$\partial_t (\psi^+ \psi) \approx - \partial_\theta j^\theta_\Omega$$

$$\Rightarrow \quad \psi^+ \psi \approx \frac{v}{\Omega r} f(r, \theta - \Omega t) + \text{const}$$

The peak of the intensity of the current across the radial direction (for individual states) is

$$I \approx e \int dr \ r \ j^\theta_\Omega \sim 10^{-1} \mu A - 1 \mu A$$

while the total intensity may be enhanced from the contribution of a large number of surface states.

The exceptional points may play an alternative role in our understanding of the topological protection of surface states in 3D semimetals.

They are behind the protection of surface states under conditions with rather large perturbations, like the case of the 3D nodal-line semimetals under strong magnetic fields.

Exceptional points may also explain the appearance of new surface states in the interaction of the 3D semimetals with the electromagnetic radiation, leading to important boundary effects.