SURFACE AND 3D QUANTUM HALL EFFECTS FROM ENGINEERING OF EXCEPTIONAL POINTS IN NODAL-LINE SEMIMETALS

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Nodal-line semimetals are characterized by having a manifold of surface states.

In a typical model of nodal-line semimetal (CaAg\(X\) (\(X = P, As\), CaP\(_3\) family)

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

the surface states adopt the form of evanescent waves

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

with well-defined pseudospin \(\sigma_y \chi = \pm \chi\)

The questions we want to address about the surface states are:

- are they transformed under the effect of a strong magnetic field?
- even if they survive, do they afford any kind of topological protection?
- are they able to support surface currents, for magnetic fields either perpendicular or parallel to the nodal ring?
TOPOLOGICAL SEMIMETALS IN STRONG MAGNETIC FIELDS

There have been already several studies of the effect of strong magnetic fields in 3D topological semimetals, showing a number of interesting signatures:

- quantum Hall effect in a Weyl semimetal with possible application in pyrochlore iridates (K.-Y. Yang et al., Phys. Rev. B 84, 075129 (2011))

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

- Landau level splitting in Cd$_3$As$_2$ under high magnetic fields (J. Cao et al., Nature Commun. 6, 7779 (2015))

- Dirac-like Landau bands in nodal-line semimetals (J.-W. Rhim and Y. B. Kim, Phys. Rev. B 92, 045126 (2015))

- 3D Hall effect in hyperhoneycomb lattices (K. Mullen, B. Uchoa and D. T. Glatzhofer, Phys. Rev. Lett. 115, 026403 (2015))
SURFACE AND 3D HALL EFFECTS IN NODAL-LINE SEMIMETALS

We take a model of nodal-line semimetal appropriate for CaAgX (X = P, As) and the CaP₃ family. For a uniform magnetic field perpendicular to the nodal ring

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

\[
\downarrow \quad A = (-By,0,0)
\]

\[
H \perp = \left( m_0 + m_1 \left( - (k_x - By)^2 + \partial_y^2 + \partial_z^2 \right) \right) \sigma_x - iv \sigma_z \partial_z
\]

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

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

\[ w = k_z + i \alpha \]

The spinor \( \chi \) must satisfy

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

The evanescent states are zero-energy modes found for \( \chi \) such that \( \sigma_y \chi = \pm \chi \), with

\[
w = k_z + i \alpha
\]

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

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

\[
w = k_z + i \alpha
\]

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

(general solution if \( 4m_0m_1 < v^2 \))
SURFACE AND 3D HALL EFFECTS IN NODAL-LINE SEMIMETALS

One can actually compute the spectrum for complex $w$

\[
\left( m_0 - m_1 \left( 2B(n + 1/2) + w^2 \right) \right) \sigma_x \chi + v w \sigma_z \chi = \varepsilon_n(w) \chi
\]

It turns out that the zero-energy eigenvalues are exceptional points in the $(k_z, \alpha)$ complex plane, that is branch points where two different branches of states coalesce.

When the model has particle-hole symmetry, $\sigma_y H \perp \sigma_y = -H \perp$, the exceptional points correspond to singular behavior $\varepsilon_n(w) \sim \pm \sqrt{w-w_i}$. One can define a topological index counting surface states from the number of exceptional points in the upper half of the complex plane

\[
\nu = \frac{1}{2\pi i} \sum_n \oint_C dw \frac{1}{\varepsilon_n(w)} \frac{d}{dw} \varepsilon_n(w)
\]

The complex structure of the spectrum lends topological protection to the zero-energy modes, since the branch cuts cannot be removed by regular perturbations.

J. G. and R. A. Molina, PRL (in press) arXiv:1710.01960
The Landau surface states do not carry in general electronic current since $j_x = -2 m_1 (k_x - B y) \sigma_x$ while the surface states have $\langle \sigma_x \rangle \approx 0$. This does not hold however when approaching the boundaries of the lateral dimension $y$:

$$\langle \sigma_x \rangle \neq 0$$

$$\langle j_x \rangle = \frac{\partial \varepsilon}{\partial k_x} \neq 0 \quad \Rightarrow \quad \sigma_{xy} = N \frac{e^2}{h}$$

J. G. and R. A. Molina, PRL (in press) arXiv:1710.01960
For a uniform magnetic field parallel to the nodal plane

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

\[ H_{\parallel} = (m_0 + m_1 \left( - (k_x + Bz)^2 - k_y^2 + \partial_z^2 \right) ) \sigma_x - iv \sigma_z \partial_z \]

The model cannot be solved exactly, but numerical resolution shows the existence of zero-energy states in the bulk localized in 2D slices parallel to the nodal plane. At \( k_x = k_y = 0 \),

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

looks like an equation for massive Dirac fermions, with two domain walls (turning points) which are able to pin a pair of evanescent waves with \( \sigma_y \chi = \pm \chi \), leading 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 section of the slab

$$\langle j_x \rangle = \frac{\partial \varepsilon}{\partial k_x} \quad \Rightarrow \quad I_x = \frac{e}{h} \int_{\text{filled states}} \frac{dk_x}{2\pi} \frac{\partial \varepsilon}{\partial k_x} \approx N \frac{e}{h} \Delta \varepsilon_F.$$ 

In terms of the maximum momentum $K_y$ at the nodal ring, the number of channels is $N = K_y \Delta y / 2\pi$.

The Hall conductivity is

$$\sigma_{zx} \approx \frac{e^2}{h} \frac{K_y}{\varepsilon_{xy} / 2\pi}.$$ 

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

The complex structure may protect the Landau surface states against perturbations (provided they preserve the particle-hole symmetry of the original model).

In thin films, there may exist a 3D Hall effect with a Hall conductance $G$ scaling linearly with the section $\Delta y$ of the sample, at a rate of a new channel per each few nanometers.