Magnetic Susceptibility of Topological Line-Node Semimetals.

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3. Line Node Semimetals
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The topological nodal semimetals are the Weyl, Dirac and line-node semimetals. In the Weyl semimetals, the electron bands contact at discrete points of the Brillouin zone and disperse linearly in all directions around these critical points. The same type of the band contact occurs in the Dirac semimetals, but the bands are double degenerate in spin, i.e., a Dirac point can be considered as a couple of the Weyl points that overlap in the quasi-momentum space. In the line node semimetals the conduction and valence bands touch along lines in the Brillouin zone and disperse linearly in directions perpendicular to these lines. There we call attention to the fact that the magnetic susceptibility $\chi$ of electrons in topological line-node semimetals should exhibit a giant anomaly. This anomaly is characterized by divergence of the magnetic susceptibility at low temperatures $T$ and weak magnetic fields $H$ when the chemical potential $\zeta$ of the electrons approaches certain critical energies $\varepsilon_c$. These critical energies correspond to the maximum and minimum values of the band-degeneracy energy in the line. We calculate $\chi$ of the line node semimetals and find dependences of $\chi$ on the $\zeta$, $T$, and $H$. 
Weyl and Dirac Semimetals.

Spectrum: $k p$ Hamiltonian.

\[
\hat{H} = \begin{pmatrix}
E_c & R & 0 & S \\
R^* & E_v & -S & 0 \\
0 & -S^* & E_c & R^* \\
S^* & 0 & R & E_v
\end{pmatrix},
\] (1)

where

\[
E_{c,v} = \varepsilon_d + v_{c,v} \cdot p,
\]

\[
R = r \cdot p,
\]

\[
S = s \cdot p.
\] (2)

- (1) takes into account a twofold spin degeneracy of electron bands in centrosymmetric crystals.
- If $S = 0$, (1) (e.g., its upper $2 \times 2$ block) describes the electron states near the Weyl points.
Weyl and Dirac Semimetals.
Spectrum: without magnetic field.

\[ \varepsilon_{c,v} = \varepsilon_d + a \cdot p + E_{c,v}, \]

\[ E_{c,v} = \pm \left\{ (a'k)^2 + |R|^2 + |S|^2 \right\}^{1/2} \]

\[ = \pm \left\{ b_{11}p_1^2 + b_{22}p_2^2 + b_{33}p_3^2 \right\}^{1/2} \]

\[ a = (v_c + v_v)/2; \quad a' = (v_c - v_v)/2. \]

can be written as

\[ \varepsilon_{c,v} = \varepsilon_d + \tilde{a} \cdot \tilde{p} \pm |\tilde{p}|, \]

where \( \tilde{p}_i = p_i \sqrt{b_{ii}} \), and \( \tilde{a}_i = a_i / \sqrt{b_{ii}} \).

- The cases \( \tilde{a}^2 < 1 \) and \( \tilde{a}^2 > 1 \) are topologically different
  (Mikitik, Sharlai, Phys. Rev. B 90, 155122, 2014)
Weyl and Dirac Semimetals.

Spectrum: Magnetic field.

\[ \varepsilon_{c,\nu}^l(p_n) = \varepsilon_d + \nu p_n \pm \left[ \frac{e\hbar\alpha H}{c} l + L \cdot (p_n)^2 \right]^{1/2}, \quad (5) \]

where

\[ \alpha = \frac{2R_n^{3/2}}{b_{11}b_{22}b_{33}\tilde{n}^2}, \]

\[ L = \frac{R_n}{b_{11}b_{22}b_{33}\tilde{n}^4}, \]

\[ R_n = \sum_{i,j=1}^{3} \kappa^{ij} n_i n_j, \quad (6) \]

\[ \kappa^{ij} = \frac{b_{11}b_{22}b_{33}}{(b_{ii}b_{jj})^{1/2}} \left[ (1 - \tilde{a}^2)\delta_{ij} + \tilde{a}_i\tilde{a}_j \right], \]

\[ \nu = \frac{(\tilde{a}\tilde{n})/\tilde{n}^2}{\tilde{n}}. \]
Weyl and Dirac Semimetals.

Magnetic susceptibility: Weak magnetic fields: $\Delta \varepsilon_H \ll T$.

\[
\chi^{ij} = -\frac{1}{6\pi^2 \hbar} \left( \frac{e}{c} \right)^2 \frac{\kappa^{ij}}{(b_{11} b_{22} b_{33})^{1/2}} \int_0^{\varepsilon_0} \frac{d\varepsilon}{\varepsilon} [f(-\varepsilon) - f(\varepsilon)], \tag{7}
\]

In the limit $T \to 0$

\[
\chi^{ij} = -\frac{1}{6\pi^2 \hbar} \left( \frac{e}{c} \right)^2 \frac{\kappa^{ij}}{(b_{11} b_{22} b_{33})^{1/2}} \ln \left( \frac{\varepsilon_0}{|\zeta - \varepsilon_d|} \right). \tag{8}
\]

At $|\zeta - \varepsilon_d| \lesssim T$

\[
\chi^{ij}(\varepsilon_d, T) = -\frac{1}{6\pi^2 \hbar} \left( \frac{e}{c} \right)^2 \frac{\kappa^{ij}}{(b_{11} b_{22} b_{33})^{1/2}} \ln \left( \frac{\varepsilon_0}{T \cdot 0.882} \right), \tag{9}
\]
Weyl and Dirac Semimetals.

Magnetic susceptibility: Strong magnetic fields: $\Delta \varepsilon_H \gg T$.

At $\zeta = \varepsilon_d$

$$\chi_{ij}(\varepsilon_d, H) = -\frac{e^2 \kappa_{ij}}{6 \pi^2 \hbar c^2 (b_{11} b_{22} b_{33})^{1/2}} \left[ A - \frac{1}{4} + \frac{1}{2} \ln \left( \frac{2\varepsilon_0^2 c}{e\hbar (1 - \tilde{\alpha}^2) R_n^{1/2} H} \right) \right]$$

If $\zeta \neq \varepsilon_d$

$$\chi_{ij} = \chi_{ij}(\varepsilon_d, H) + \delta \chi_{ij}$$

$$\delta \chi_{ij} = \frac{e^2}{2 \pi^2 c^2 \hbar} \frac{\kappa_{ij}}{(b_{11} b_{22} b_{33})^{1/2}} \left\{ u + 2 \sum_{m=1}^{M} \left[ \sqrt{u(u - m)} - 2m \cdot \ln \left( \frac{\sqrt{u} + \sqrt{u - m}}{\sqrt{m}} \right) \right] \right\}, \quad (10)$$

where

$$u \equiv \frac{(\zeta - \varepsilon_d)^2 c}{2e\hbar(1 - \tilde{\alpha}^2) R_n^{1/2} H} = \frac{S_{ex} c}{2\pi \hbar eH}, \quad (11)$$
Line-Node Semimetals.
Spectrum in the vicinity of a band-contact line.

\[
\varepsilon_{c,v} = \varepsilon_d(p_3) + a_\perp p_\perp \pm E_{c,v},
\]

\[
E_{c,v}^2 = b_{11}p_1^2 + b_{22}p_2^2,
\]
Line-Node Semimetals.
Spectrum. Magnetic field.

\[ \varepsilon_{c,v}^l(p_3) = \varepsilon_d(p_3) \pm \left( \frac{e\hbar \alpha H |\cos \theta|}{c} \right)^{1/2}, \]  

(13)

where \( \alpha = \alpha(p_3) = 2(b_{11} b_{22})^{1/2}(1 - \tilde{a}_\perp^2)^{3/2}. \)

Below, the Example model,

- Spectrum \( \varepsilon_d(p_3) = \varepsilon_d^0 + \Delta \cos(2\pi p_3 n/L). \)
- Band-contact line is approximately a circle.
Line-Node Semimetals.

Magnetic susceptibility: Weak magnetic fields: $\Delta \varepsilon_H \ll T$.

$$\chi_{||} = \frac{e^2}{6\pi^2 \hbar c^2} \int_0^L dp_3 (b_{11} b_{22})^{1/2} \left(1 - \tilde{a}_\perp^2\right)^{3/2} f'(\varepsilon_d) \cos^2 \theta, \quad (14)$$

At $T \ll 2\Delta$

$$\chi_{||}(\zeta) = -\frac{e^2}{6\pi^2 \hbar c^2} \sum_j (b_{11} b_{22})^{1/2} (1 - \tilde{a}_\perp^2)^{3/2} \frac{\cos^2 \theta}{|d\varepsilon_d/dp_3|}, \quad (15)$$

for $p_3 = p_{3j}$, where $\varepsilon_d(p_{3j}) = \zeta$.

In the Example Model, $p_{3j} = \pm \frac{L}{2\pi n} \arccos \left(\frac{\zeta - \varepsilon_0^d}{\Delta}\right)$, and

$$\chi_{||}(\zeta) = -\frac{e^2}{6\pi^2 \hbar c^2} \frac{L (b_{11} b_{22})^{1/2} (1 - \tilde{a}_\perp^2)^{3/2} \cos^2 \theta_0}{2\pi \sqrt{\Delta^2 - (\zeta - \varepsilon_0^d)^2}}, \quad (16)$$
Line-Node Semimetals.

Magnetic susceptibility: Weak magnetic fields: $\Delta \varepsilon_H \ll T$. Plots.

The dependence of $\chi_\parallel$ on the chemical potential $\zeta$ at

1) $T \to 0$
2) $T/\Delta = 0.25$
3) $T/\Delta = 2$
Line-Node Semimetals.
Magnetic susceptibility: Strong magnetic fields: $\Delta \epsilon_H \gg T$.

General expression for any $H$:

$$
\chi_{\parallel}(\zeta, H) = \frac{e^{3/2}H^{-1/2}}{2\pi^2\hbar^{3/2}c^{3/2}} \int_0^L dp_3 |\cos \theta|^{3/2} \sqrt{\alpha(p_3)} K(u),
$$

where

$$
\alpha(p_3) = 2(b_{11} b_{22})^{1/2}(1 - \tilde{a}_\perp^2)^{3/2},
$$

$$
K(u) = \frac{3}{2} \zeta(-\frac{1}{2},[u]+1) + \sqrt{u}([u] + \frac{1}{2}).
$$

$\zeta(x, a)$ is the Hurwitz zeta function, $[u]$ is the integer part of $u$,

$$
u = \frac{[\zeta - \epsilon_d(p_3)]^2 c}{e\hbar \alpha(p_3) H |\cos \theta|} = \frac{cS(p_3)}{2\pi e\hbar H},
$$
If the chemical potential $\zeta$ tends to one of the critical energies $\varepsilon^0_d \pm \Delta$,

$$
\chi_{\parallel}(H) = -\frac{f_0 e^{7/4} \alpha_c^{3/4} n}{\pi^2 \hbar^{5/4} c^{7/4} |B|^{1/2}} \cdot H^{-1/4} (\cos \theta_0)^{7/4} \Phi_n(\phi),
$$

(19)

where $f_0 \approx 0.156$, $\alpha_c$ denotes the value of $\alpha$ at one of the critical points, the factor $\Phi_n(\phi)$,

$$
\Phi_n(\phi) = \frac{1}{n} \sum_{i=1}^{n} \left| \cos \left( \phi + \frac{2\pi i}{n} \right) \right|^{7/4},
$$

(20)
Line-Node Semimetals.

Magnetic susceptibility: Strong magnetic fields: $\Delta \varepsilon_H \gg T$. Approximations 2/2.

If the magnetic field be so large that $\Delta \ll \Delta \varepsilon_H$:

$$
\chi_{\parallel}(\zeta, H) \approx \frac{3e^{3/2}H^{-1/2}}{4\pi^2\hbar^{3/2}c^{3/2}} \zeta(-\frac{1}{2}, 1)(\cos \theta_0)^{3/2}G_{\parallel}(\phi)
$$

\[+\frac{e \cos \theta_0}{4\pi^2\hbar^2 cH} \int_0^L dp_3 |(\zeta - \varepsilon_d(p_3)) \cos \varphi(p_3)|, \quad (21)\]

where

$$
G_{\parallel}(\phi) = \int_0^L dp_3 |\cos \varphi(p_3)|^{3/2} \sqrt{\alpha(p_3)}, \quad (22)
$$
The $H$-dependence of the quantity $M_{\parallel}/H$ calculated at $\alpha = \text{const}$, $T = 0.25\Delta$ for the three values of the chemical potential $\zeta$ measured from $\varepsilon^0_d$.

- 1) $\zeta = 0$
- 2) $\zeta = \Delta$
- 3) $\zeta = 1.5\Delta$
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