Phase Diagram and Chiral Magnetic Effect in Dirac Semimetals from Lattice Simulation

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arXiv:1608.07162, Phys.Rev. B94 (2016) no.20, 205147
arXiv:1704.07132
and ‘in preparation

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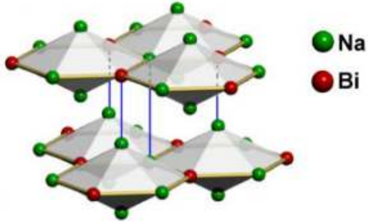
Dirac semimetals

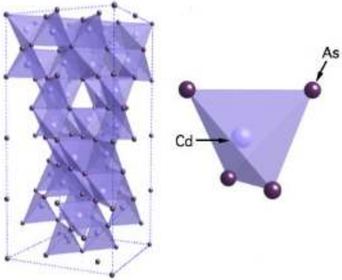
- Condensed matter analog of QGP
  - strongly coupled
  - massless fermions
- $3D$ analog of graphene ($2D$)
- Perfect toolkit for tabletop study of phenomena, previously attributed to HEP (e.g. anomalous transport)

Dirac semimetals. Elementary structure



Na_3Bi

arXiv:1310.0391, Z. K. Liu et al.

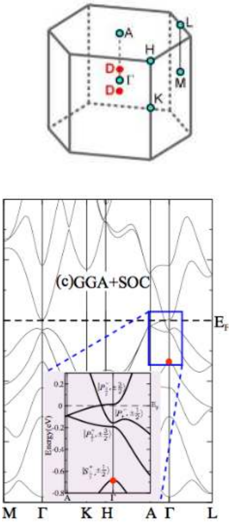


Cd_3As_2

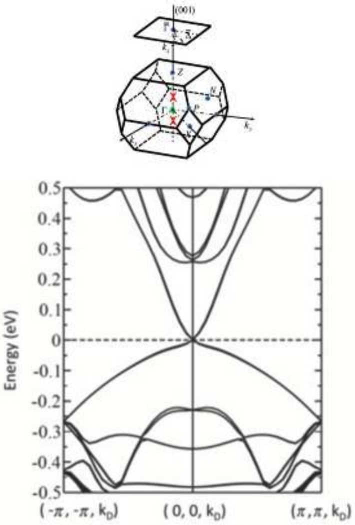
arXiv:1309.7892, M. Neupane et al.

arXiv:1309.7978, S. Borisenko et al.

Band structure

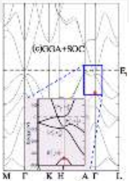


Na$_3$Bi



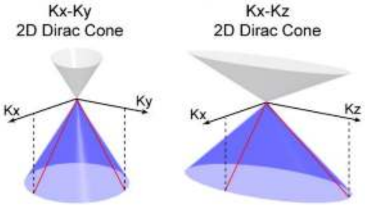
Cd$_3$As$_2$

How to study these materials?



Effective theory approach

- Relevant energy scales
- Relevant degrees of freedom



arXiv:1310.0391, Z. K. Liu et al.

$N = 2$ Dirac points in electronic dispersion

$$E \sim \sqrt{v_\perp^2 (k_x^2 + k_y^2) + v_\parallel^2 k_z^2}$$

Effective theory

- $N = 2$ Massless Dirac fermions
- Fermi velocity is $v_f \ll c$
- Anisotropy in Fermi velocity $v_{\parallel} \neq v_{\perp}$

  effectively induced by strain (arXiv:1609.00615, S.Guan et al.)
- Electromagnetic interaction
- Effective charge is $\alpha_F = \frac{\alpha}{v_F} \sim 1$, $\alpha = \frac{1}{137}$

$$Z = \int D\bar{\psi} D\psi DA \exp\Big(-\frac{1}{8\pi\alpha_F}\int d^4x[\partial_j A_4]^2 +$$
$$i\int d^4x \bar{\psi}\Big(\gamma^4[\partial_4 + iA^4] + \xi_k\gamma^k\partial_k\Big)\psi\Big)$$

Lattice discretization

Staggered fermions ($N = 4 \to N = 2$ via rooting):

$$S_{\Psi int.} = \sum_x m\bar{\Psi}_x\Psi_x + \frac{1}{2}\sum_{i=1,2,3}\xi_i(\bar{\Psi}_x\alpha_{x,i}\Psi_{x+\hat{i}} - \bar{\Psi}_x\alpha_{x,i}\Psi_{x-\hat{i}}) +$$

$$+\frac{1}{2}\bar{\Psi}_x\alpha_{x,4}\exp(i\theta_{l,4}(x))\Psi_{x+\hat{4}} - \frac{1}{2}\bar{\Psi}_x\alpha_{x,4}\exp(-i\theta_{l,4}(x-\hat{4}))\Psi_{x-\hat{4}}$$

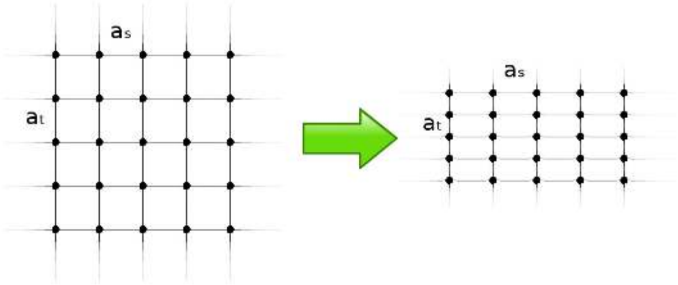
Noncompact gauge action:

$$S_g = \frac{\beta}{2}\sum_{i=1,2,3}\theta^2_{p,\hat{i}4}(x), \beta = \frac{1}{4\pi\alpha_F}$$

$$\theta_{p,\hat{i}4} = \theta_{l,4}(x+\hat{i}) - \theta_{l,4}(x)$$

Lattice discretization

Different time- and space- like steps: $a_s \neq a_t$



The same idea was in PoS LATTICE2015, 046 (2016), Y. Araki.

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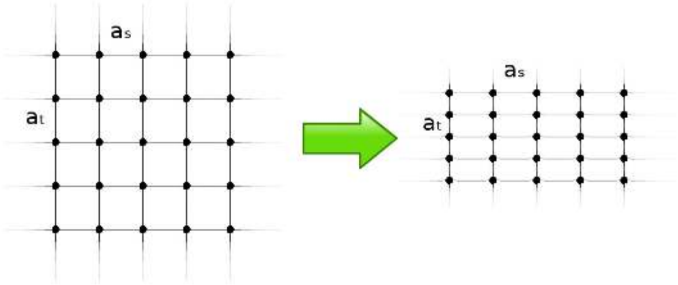

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Hamiltonian approach($a_t \to 0$):

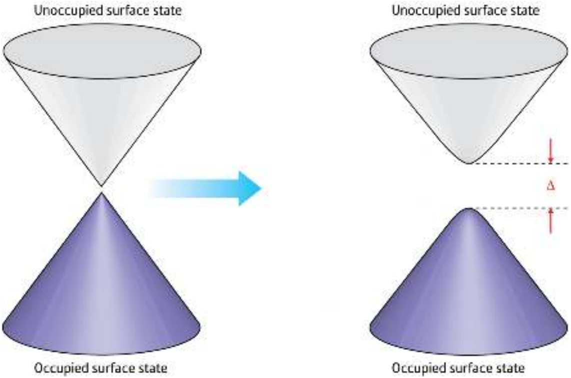
- Rooting $N_f : 4 \to 2$ (taste breaking $\sim a_t^2(\gamma_5 \otimes \gamma_5\gamma_4^T)\delta_4 \to 0$)

  more details in arXiv:1704.07132

- Small FV effects
- More freedom in varying T, eB

Phase diagram. Semimetal - Insulator transition.

At large enough α gapped phase?

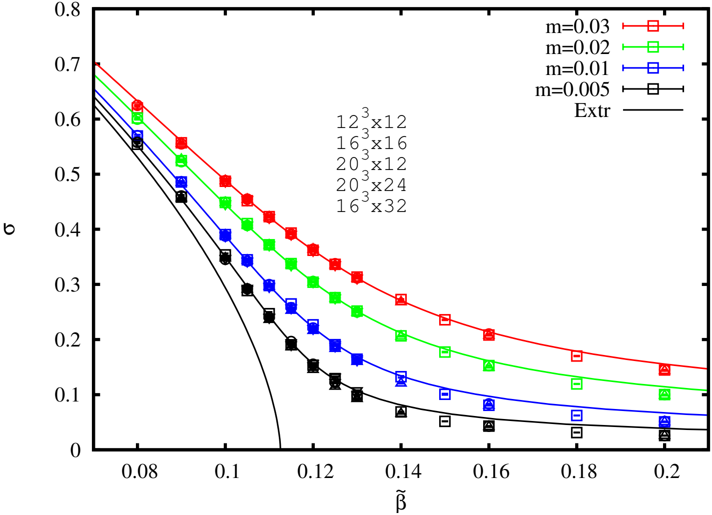


Is there a gap? What is the value of α_c?
Order parameter:

$$\sigma = \langle \bar{\psi}\psi \rangle = \frac{1}{V}\langle \mathrm{tr}\, D^{-1} \rangle$$

Isotropic case $v_{F,x} = v_{F,y} = v_{F,z} = v_F$.

$\xi_i = v_F \frac{a_t}{a_s} = \frac{1}{2}$



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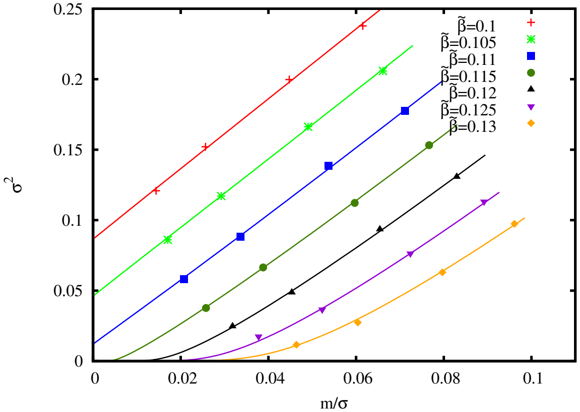
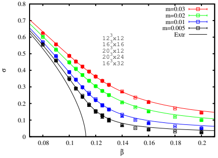
$\xi_i = v_F \frac{a_t}{a_s} = \frac{1}{2}$ $\quad 16^3 \times 16$

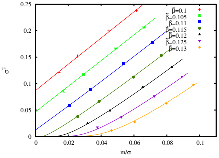


Equation of State (motivated by QED & graphene):
$m(X_0 + X_1(1 - \beta/\beta_c)) = \sigma^\delta + Y_1(1 - \beta/\beta_c)\sigma^b$.
Classical: $\delta = 3,\ b = 1$.

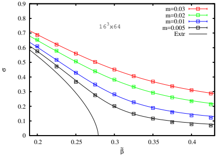
Isotropic case $v_{F,x} = v_{F,y} = v_{F,z} = v_F$.

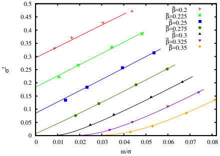
$\xi_i = \frac{1}{2}$



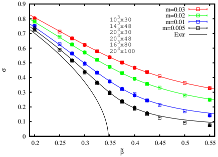


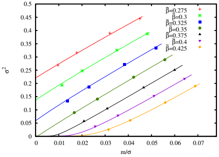
$\xi_i = \frac{1}{4}$



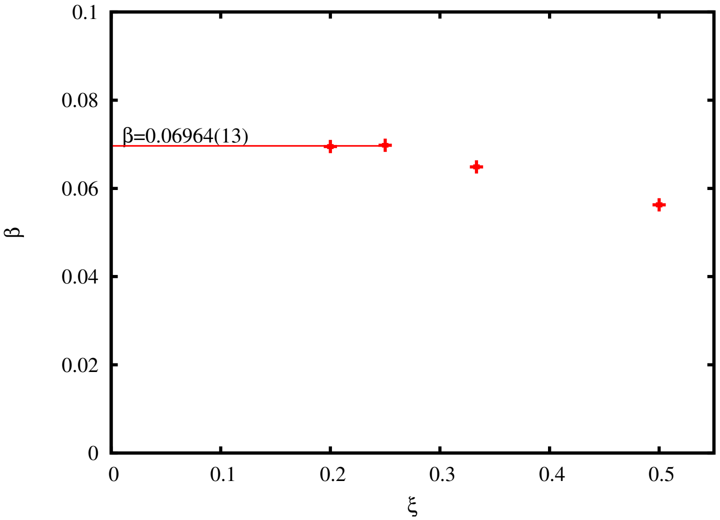


$\xi_i = \frac{1}{5}$





Isotropic case $v_{F,x} = v_{F,y} = v_{F,z} = v_F$.



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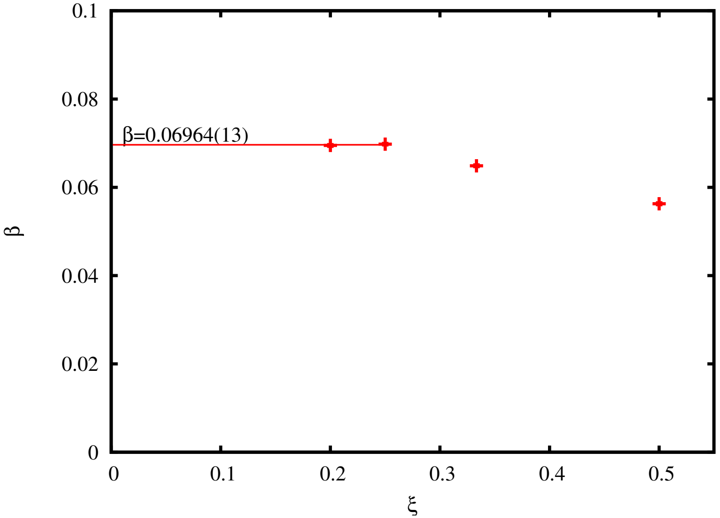


$\beta_c \sim 0.069 \rightarrow \alpha_c \sim 1.14$

$\alpha_c \approx 1.8660$, J.Gonzalez, arXiv:1509.00210, Ladder approximation

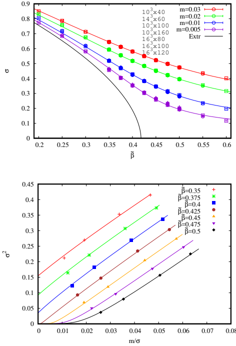
Anisotropy in Fermi velocity

- $v_{F,1} = v_{F,2} = v_F$
- $v_{F,3} = \zeta v_F$, ζ is varied
- $\beta = \frac{v_F}{4\pi e^2}$

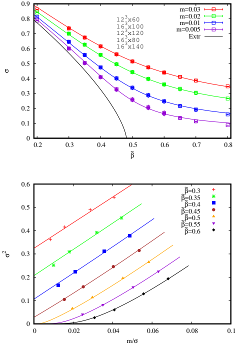
Lattice:

- $\xi_1 = \xi_2 = \xi = \frac{1}{5}$
- $\xi_3 = \zeta\xi$
- $\beta = \tilde{\beta}\xi$

Anisotropy in Fermi velocity



$\zeta = \frac{1}{2}$



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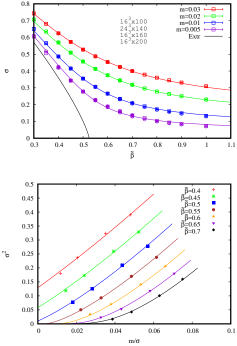
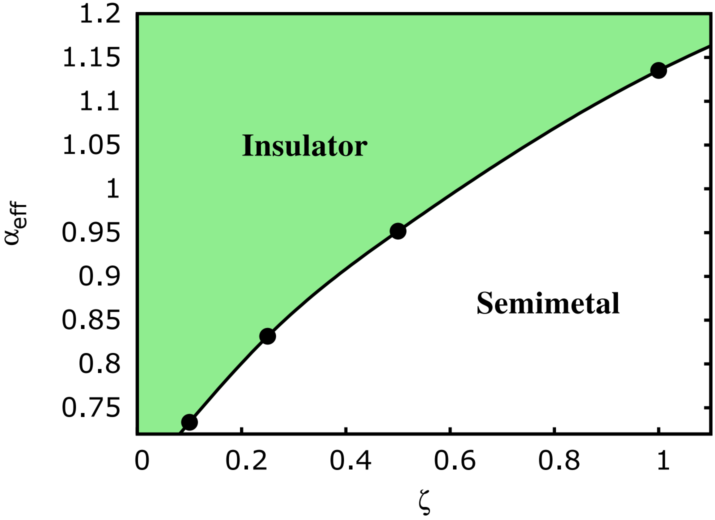


$\zeta = \frac{1}{10}$

Phase diagram



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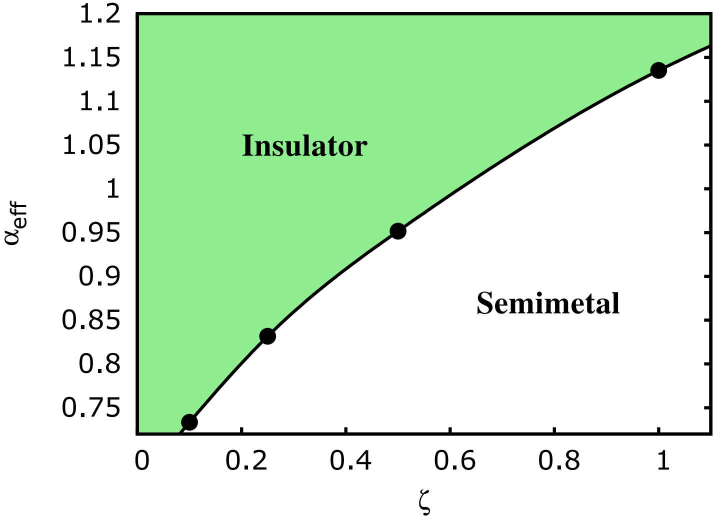
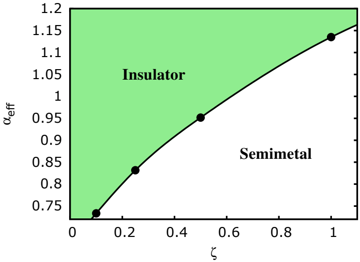


$\zeta : 1 \to 0 \Longrightarrow 3D \to 2D$

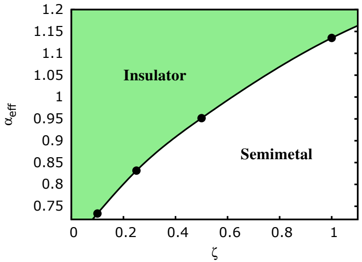
Phase diagram



- Na_3Bi: $\alpha_{eff} \approx 7$
- Cd_3As_2: $\alpha_{eff} \approx 2$

Both should be in insulator phase!

Phase diagram



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Possible solutions:

- Screening by bound electrons(ϵ)
- Renormalization

Chiral Magnetic Effect

Conductivity in external magnetic field

Chiral magnetic effect(CME) in Dirac semimetals:

- $\vec{E} \parallel \vec{B}$

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$\rho_5(\mu_5)$?

- Small B: $\rho_5 \sim \mu_5 T^2 \Longrightarrow \sigma_{\parallel} \sim B^2$
- Large B: $\rho_5 \sim \mu_5 B \Longrightarrow \sigma_{\parallel} \sim B$

Conductivity on the lattice

Kubo relation ($K(\omega, t) = \frac{2\omega \cosh(w(\frac{1}{2T} - t))}{\sinh(\frac{\omega}{2T})}$):

$$\int d^3\bar{x} \langle j_i(\bar{x}, t) j_i(0) \rangle = \int_0^\infty \frac{d\omega}{2\pi} K(\omega, t) \sigma_i(\omega),$$

In the middle point:

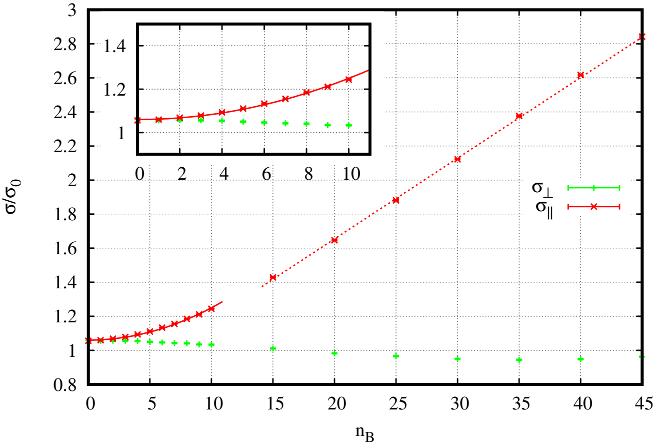
$$C_i(\frac{1}{2T}) = \int_0^\infty \frac{d\omega}{2\pi} \frac{2\omega}{\sinh \frac{\omega}{2T}} \sigma_i(\omega)$$

Estimation:

$$\sigma_i^{(0)} = \int_0^\infty \frac{d\omega}{2\pi} \frac{2\omega}{\sinh \frac{\omega}{2T}} \sigma_i(\omega) / \int_0^\infty \frac{d\omega}{2\pi} \frac{2\omega}{\sinh \frac{\omega}{2T}} = \frac{1}{\pi T^2} C_i(\frac{1}{2T})$$

Conductivity in external magnetic field

$\beta = 0.25$ (Semimetal phase) Lattice 20^4 $a_t/a_s = 1/4$



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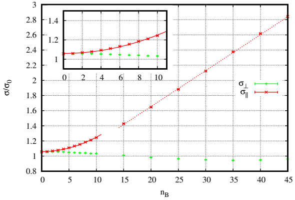
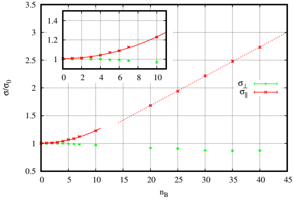
Conductivity(different phases)

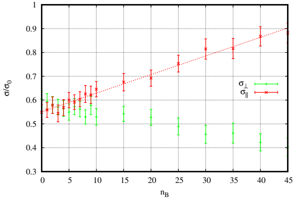
SM
$\beta = 0.25$

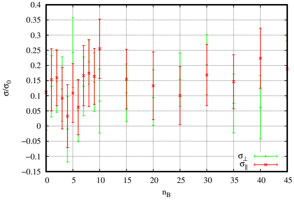




SM
$\beta = 0.125$

Transition
$\beta = 0.0625$

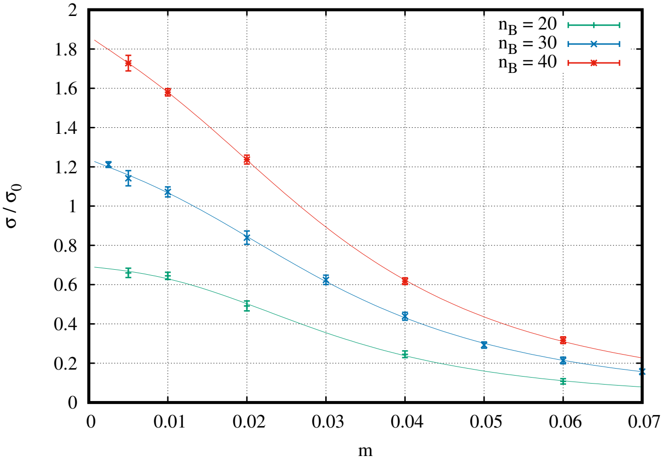




Insulator
$\beta = 0.03125$

CME Conductivity $\sigma_{\parallel}(B) - \sigma_{\parallel}(0)$ vs mass

$\beta = 0.25$ (Semimetal phase) Lattice 20^4 $a_t/a_s = 1/4$



$$\sigma(m) = \frac{\tilde{\sigma}_0}{m + \alpha m^3 \log(m) + \gamma}$$

Conclusions

- Lattice Formulation and Study of Dirac semimetals
- $\frac{a_t}{a_s} \to 0$ is crucial
- Semimetal-insulator transition in Dirac semimetals
- Observed DSM should be insulating
- Screening? Renormalization?
- We observe Chiral Magnetic Effect