Numerical simulation of Dirac semimetals

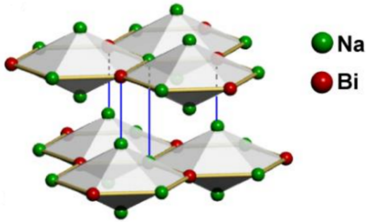
Workshop "Condensed matter physics meets relativistic quantum field theory"

15 Jun, 2016

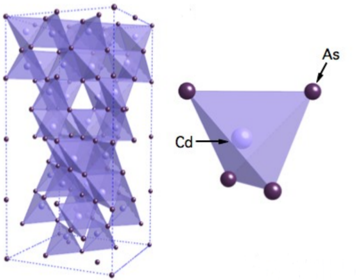
QCD, Graphene and Dirac semimetals

QCD	Graphene	Dirac semimetals
Quarks Confinement-Deconfinement Chiral condensate	Massless fermions Insulator-semimetal Fermion condensates	

Dirac semimetals. Elementary structure

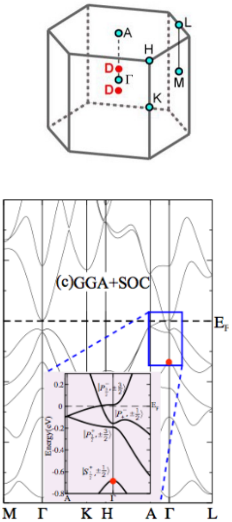


Na_3Bi
arXiv:1310.0391, Z. K. Liu et al.

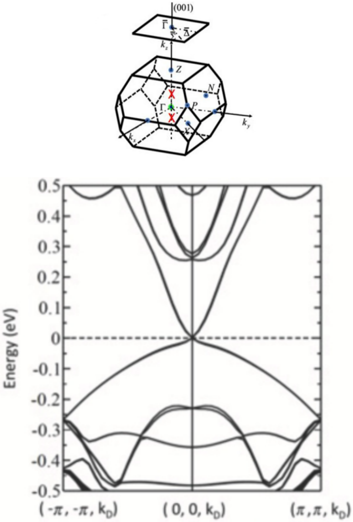


Cd_3As_2
arXiv:1309.7892, M. Neupane et al.
arXiv:1309.7978, S. Borisenko et al.

Band structure

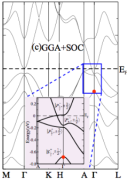


Na_3Bi



Cd_3As_2

Take into account all energy levels?

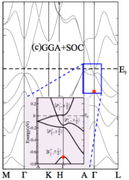


How to study these materials?

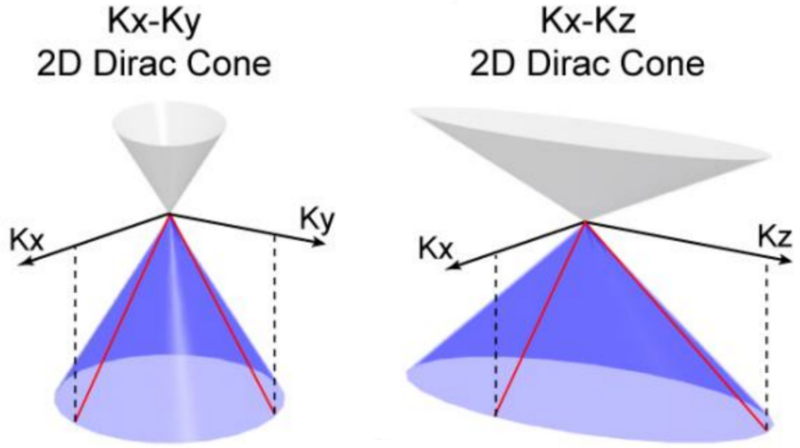
Take into account all energy levels?

Effective theory approach

- Relevant energy scales
- Relevant degrees of freedom



Dirac points



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 $v_f \sim c/200$
- Anisotropy in Fermi velocity $v_\parallel \neq v_\perp$
- Effective charge is $\alpha_F = \frac{\alpha}{\epsilon v_F}$

Effective theory

- Low-energy effective theory: fermionic quasiparticles
- Interaction with electromagnetic field

$$
\begin{aligned}
Z \;&=\; \int D\bar{\psi} D\psi DA \exp\Big(-i \frac{1}{4g^2} \int d^3x dt F_{\mu\nu} F^{\mu\nu} + \\
& i \int d^3x dt \, \bar{\psi}_a [i\partial_\mu - A_\mu] \gamma^b e_b^\mu \psi_a \Big)
\end{aligned}
$$

$$
e_b^\mu \sim \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & v_\perp & 0 & 0 \\ 0 & 0 & v_\perp & 0 \\ 0 & 0 & 0 & v_\parallel \end{pmatrix}
$$

Effective theory

- Low-energy effective theory: fermionic quasiparticles
- Interaction with electromagnetic field

$$Z = \int D\bar{\psi} D\psi DA \exp\Big(-i\frac{1}{4g^2}\int d^3x dt F_{\mu\nu}F^{\mu\nu} + i\int d^3x dt\, \bar{\psi}_a[i\partial_\mu - A_\mu]\gamma^b e^\mu_b \psi_a\Big)$$

$$e^\mu_b \sim \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & v_\perp & 0 & 0 \\ 0 & 0 & v_\perp & 0 \\ 0 & 0 & 0 & v_\parallel \end{pmatrix}$$

It allows to apply methods of (lattice) field theory!

Field theory of Dirac semimetals

Partition function

$$Z = \int D\bar{\psi} D\psi DA \exp\Big(-i\frac{1}{4g^2}\int d^3x dt F_{\mu\nu}F^{\mu\nu} + i\int d^3x dt\, \bar{\psi}_a[i\partial_\mu - A_\mu]\gamma^b e^\mu_b \psi_a\Big)$$

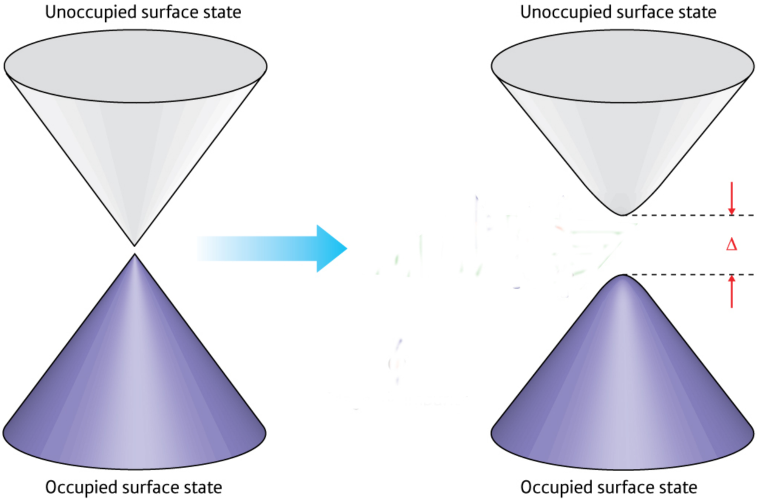
$$t \to -ix^4/v_F \quad A^0 \to -iv_F A^4 \quad A_j \to \frac{1}{\sqrt{v_F}}A_j$$

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

$$\alpha_F = \frac{\alpha}{\epsilon v_F}$$

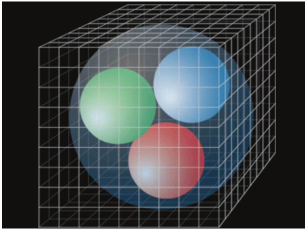
Semimetal - Insulator transition

At large enough α gapped phase?



Is there a gap? What is the value of β_c?

Lattice field theory approach



- QCD, QED
- Graphene
  J.E. Drut, T.A. Lahde
  P.V. Buividovich, O.V. Pavlovsky, M.V.Ulybyshev,
  E.V. Luschevskaya, M.A. Zubkov, V.V. Braguta,
  M.I. Polikarpov
- Dirac semimetals

Lattice discretization

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

$$S_{\Psi int.} = \sum_x m\bar{\Psi}_x\Psi_x + \frac{1}{2}\sum_{i=1,2,3}\xi_i(\bar{\Psi}_x\alpha_{x,i}\Psi_{x+\hat{\imath}} - \bar{\Psi}_x\alpha_{x,i}\Psi_{x-\hat{\imath}}) +$$
$$+\frac{1}{2}\bar{\Psi}_x\alpha_{x,4}\exp(i\theta_{l,4}(x))\Psi_{x+\hat{4}} - \frac{1}{2}\bar{\Psi}_x\alpha_{x,4}\exp(-i\theta_{l,4}(x-\hat{4}))\Psi_{x-\hat{4}}$$

Noncompact gauge action:

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

Lattice strategy

- Hybrid Monte-Carlo
- Lattice size 20^4
- $N = 2$ dynamical staggered fermions
- Chiral limit $m \to 0$
- $\xi_1 = \xi_2 = 1$, different ξ_3

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

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

Observables

- Order parameter for semimetal-insulator phase transition (chiral condensate):

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

- Susceptibility:

$$\chi = \frac{\partial \sigma}{\partial m} = \frac{1}{V}(\langle \mathrm{tr}^2\, D^{-1} \rangle - \langle \mathrm{tr}\, D^{-2} \rangle - \langle \mathrm{tr}\, D^{-1} \rangle^2)$$

- Logarithmic derivative:

$$R = \frac{\partial \log \sigma}{\partial \log m} = \frac{m}{\sigma}\chi$$

Observables

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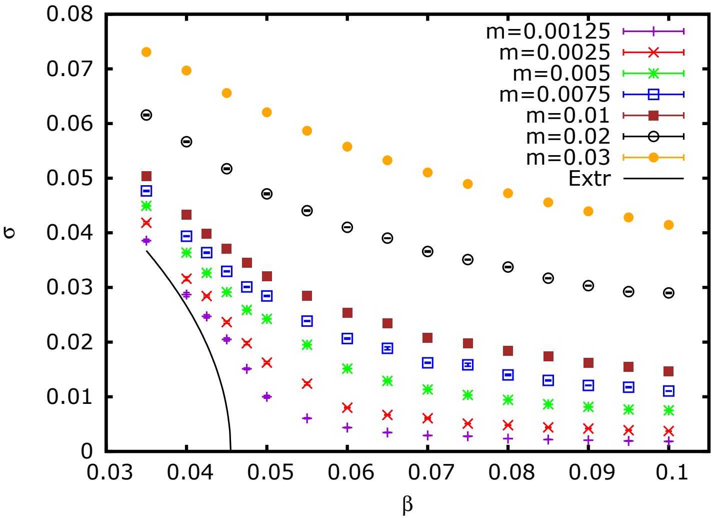
- Logarithmic derivative:

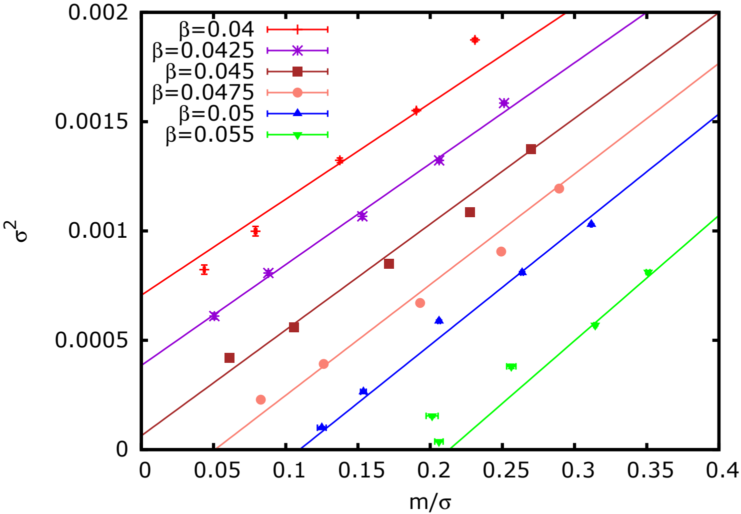
$$R = \frac{\partial \log \sigma}{\partial \log m} = \frac{m}{\sigma} \chi$$

χS	Broken	Restored
σ	$\sim$ *const*	$\sim m \to 0$
χ	Peak at the transition	
R	0	1

$\xi = 1$. Condensate



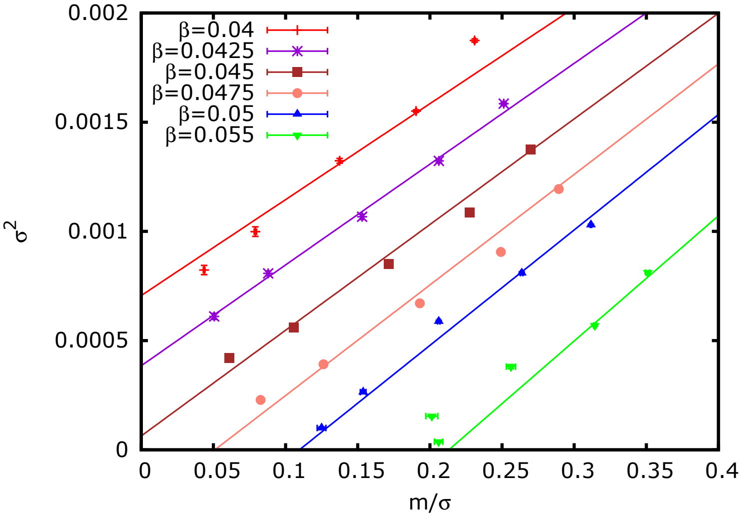
$\xi = 1$. Fisher plot



Equation of State (motivated by QED):

$m(X_0 + X_1(1 - \beta/\beta_c)) = \sigma^3 + Y_1(1 - \beta/\beta_c)\sigma.$

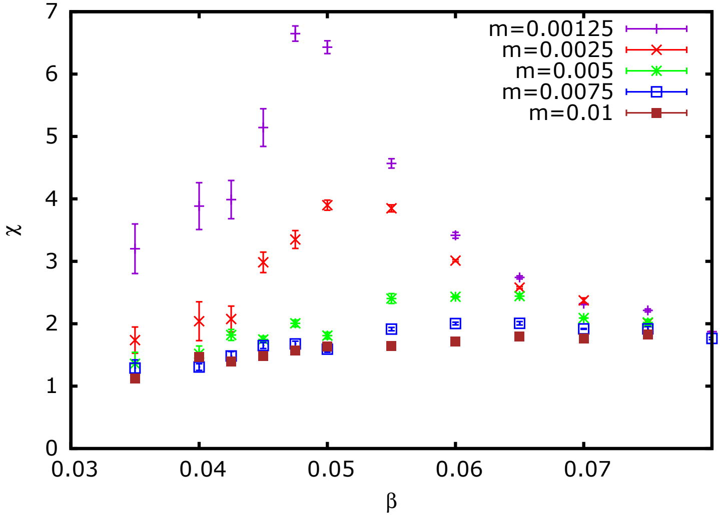
$\xi = 1$. Fisher plot



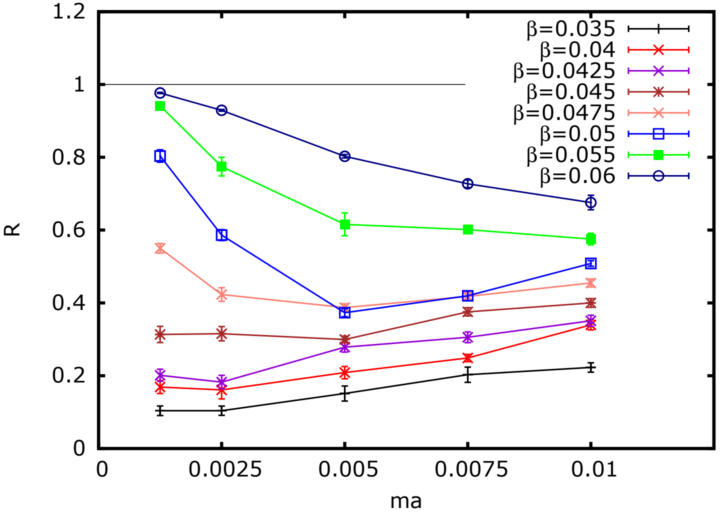
$\beta_c \sim 0.045 \to \alpha_c \sim 1.76$

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

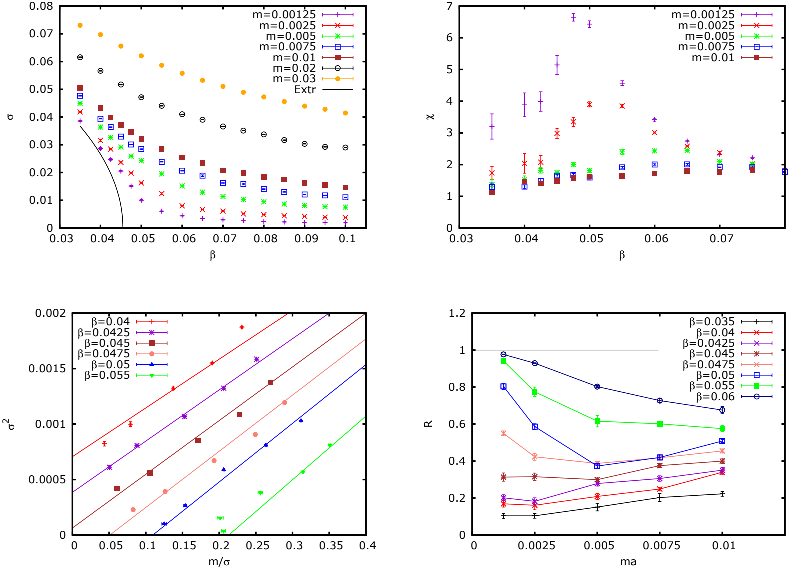
$\xi = 1$. Susceptibilities



$\xi = 1$. Logarithmic derivative

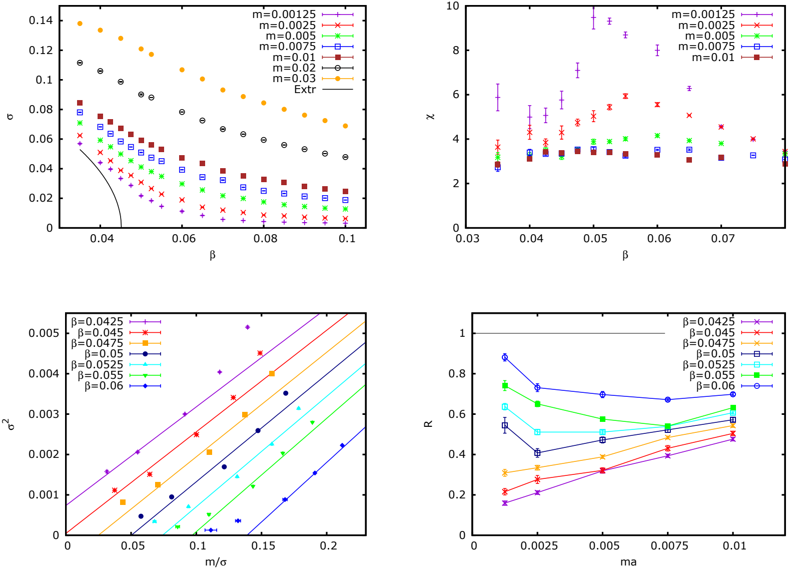


$\xi = 1$



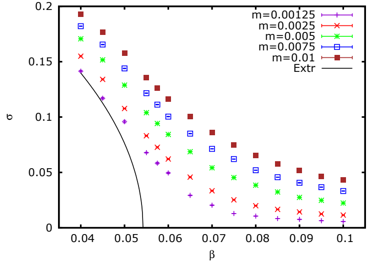
m=0.00125
m=0.0025
m=0.005
m=0.0075
m=0.01
m=0.02
m=0.03
Extr
σ
β
χ
β=0.04
β=0.0425
β=0.045
β=0.0475
β=0.05
β=0.055
σ²
m/σ
β=0.035
β=0.06
R
ma

$\xi = 0.5$

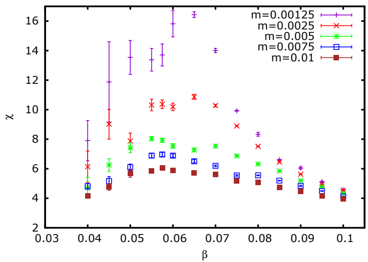


m=0.00125
m=0.0025
m=0.005
m=0.0075
m=0.01
m=0.02
m=0.03
Extr
σ
β
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
0.04
0.06
0.08
0.1
χ
10
8
6
4
2
0.03
0.05
0.07
σ^2
m/σ
β=0.0425
β=0.045
β=0.0475
β=0.05
β=0.0525
β=0.055
β=0.06
0.005
0.004
0.003
0.002
0.001
0.15
0.2
R
ma
1
0.8
0.6
0.4
0.2
0.0025
0.005
0.0075
0.01

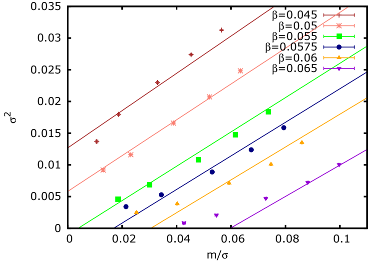
$\xi = 0.2$



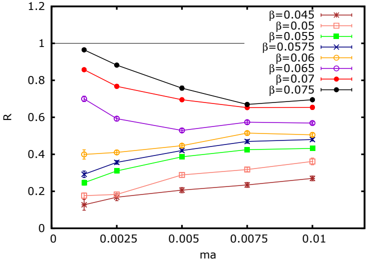
σ
β
m=0.00125
m=0.0025
m=0.005
m=0.0075
m=0.01
Extr



χ
β
m=0.00125
m=0.0025
m=0.005
m=0.0075
m=0.01

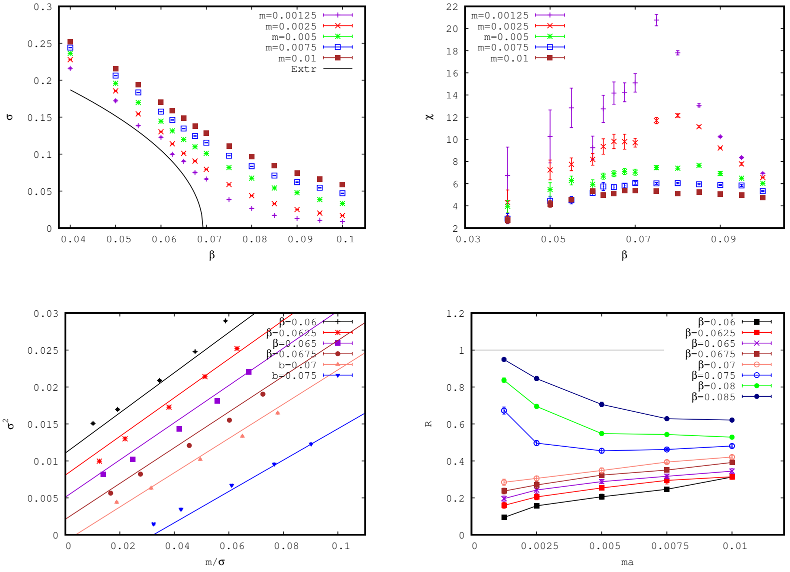


σ²
m/σ
β=0.045
β=0.05
β=0.055
β=0.0575
β=0.06
β=0.065

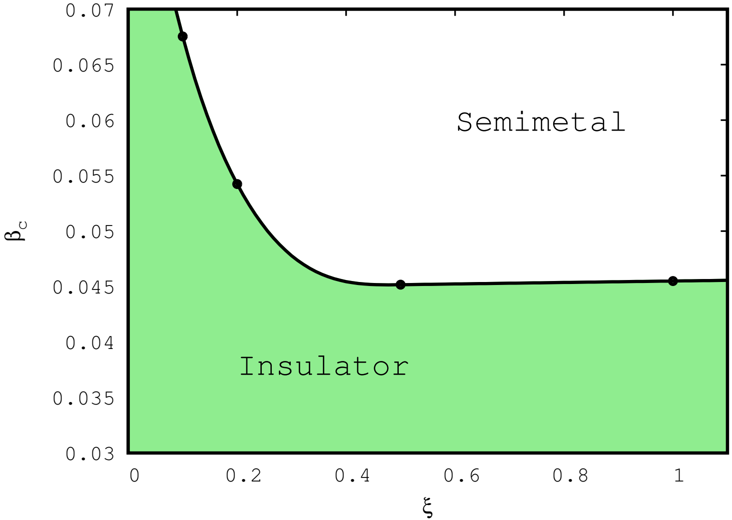


R
ma
β=0.045
β=0.05
β=0.055
β=0.0575
β=0.06
β=0.065
β=0.07
β=0.075

$\xi = 0.1$



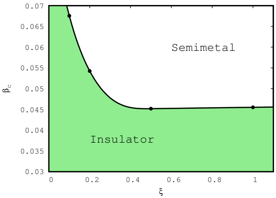
σ
β
m=0.00125
m=0.0025
m=0.005
m=0.0075
m=0.01
Extr
χ
β
m=0.00125
m=0.0025
m=0.005
m=0.0075
m=0.01
σ²
m/σ
β=0.06
β=0.0625
β=0.065
β=0.0675
b=0.07
b=0.075
R
ma
β=0.06
β=0.0625
β=0.065
β=0.0675
β=0.07
β=0.075
β=0.08
β=0.085



0.07
0.065
0.06
0.055
0.05
0.045
0.04
0.035
0.03
β_c
0
0.2
0.4
0.6
0.8
1
ξ
Semimetal
Insulator

Conclusions

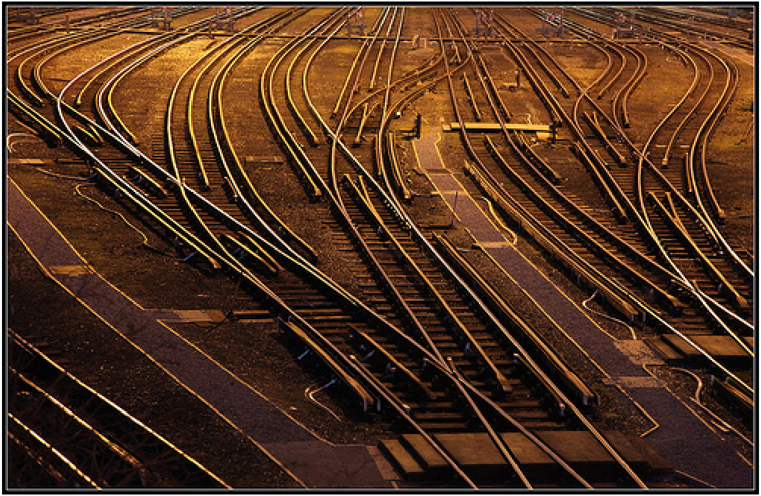
- First results of study of Dirac semimetals by means of lattice field theory
- Semimetal-insulator transition in Dirac semimetals
- β_c grows if we increase asymmetry
- Dimensional reduction
- $L \to \infty$?



Field theory approach

Within lattice field theory approach one can study:

- Phase diagram
- Magnetic field
- Temperature
- Impurities, deformations
- (Anomalous) transport phenomena and properties
- Chiral effects
- ...



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