Numerical simulation of Dirac semimetals

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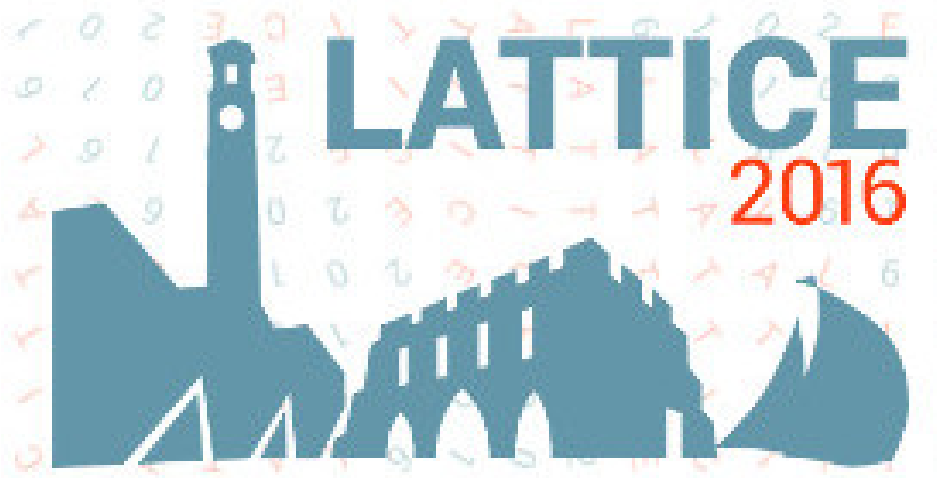
34th International Symposium on Lattice Field Theory

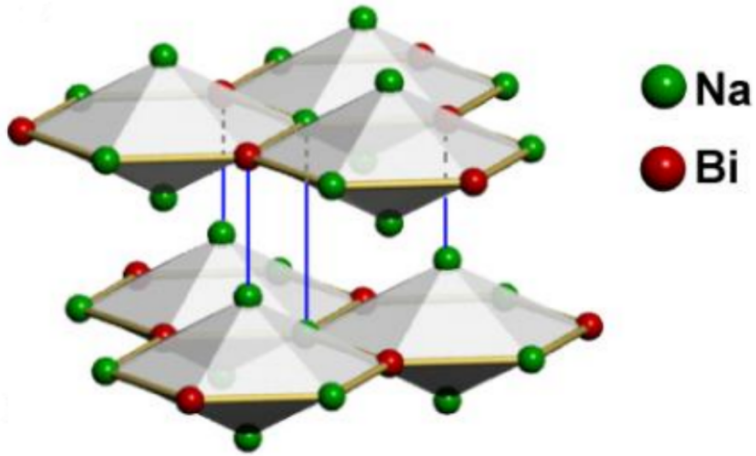


24-30 Jul, 2016

Dirac semimetals

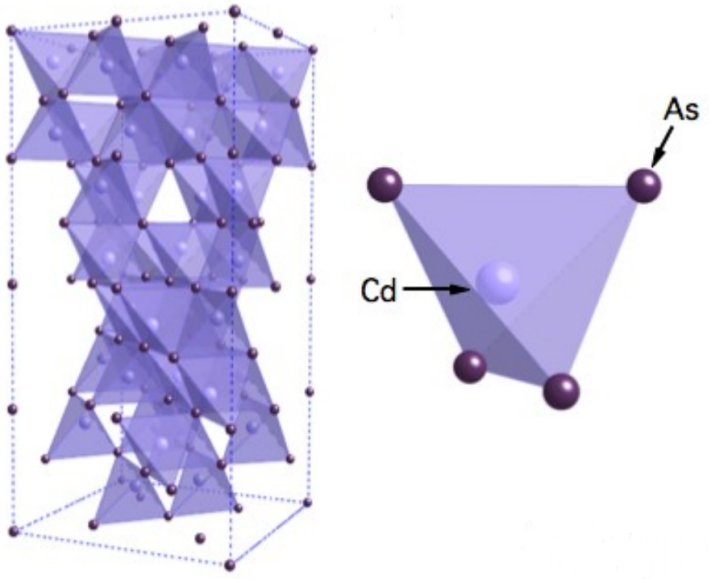
- Condensed matter analog of QGP
  - strongly coupled
  - massless fermions
- $3D$ analog of graphene ($2D$)

Dirac semimetals. Elementary structure



Na_3Bi

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

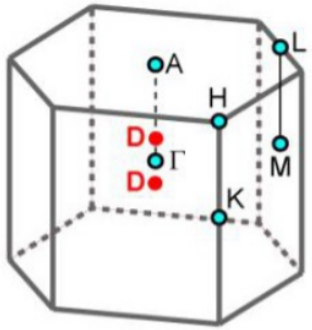


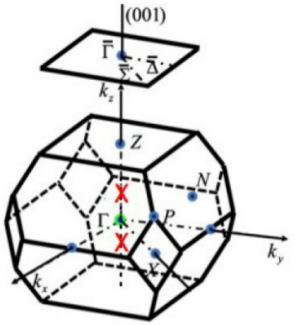
Cd_3As_2

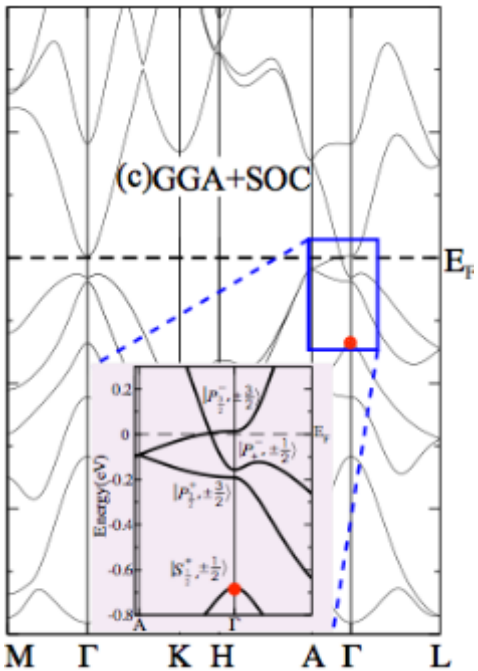
arXiv:1309.7892, M. Neupane et al.

arXiv:1309.7978, S. Borisenko et al.

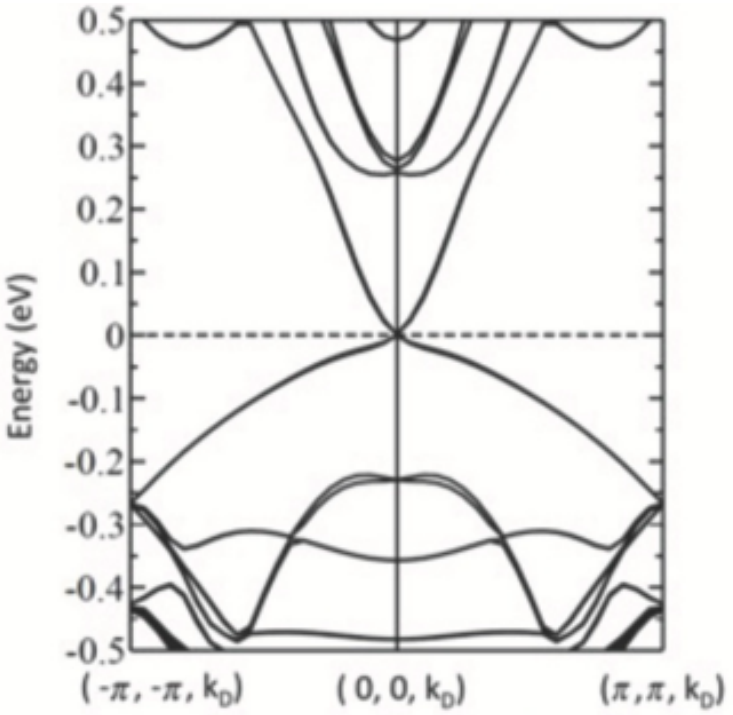
Band structure







Na_3Bi



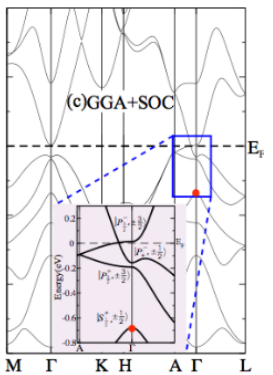
Cd_3As_2

How to study these materials?

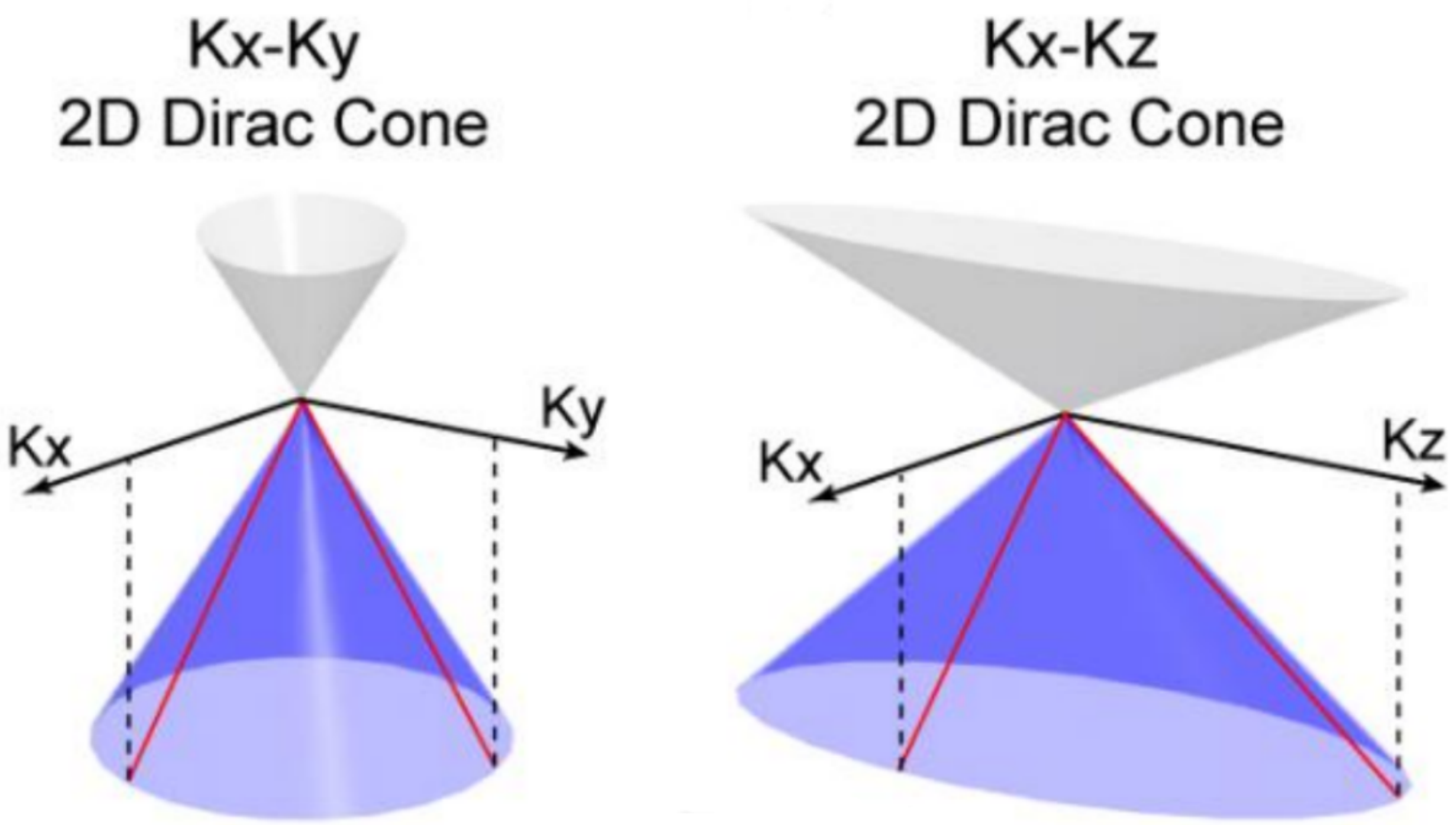
Take into account all energy levels?

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

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

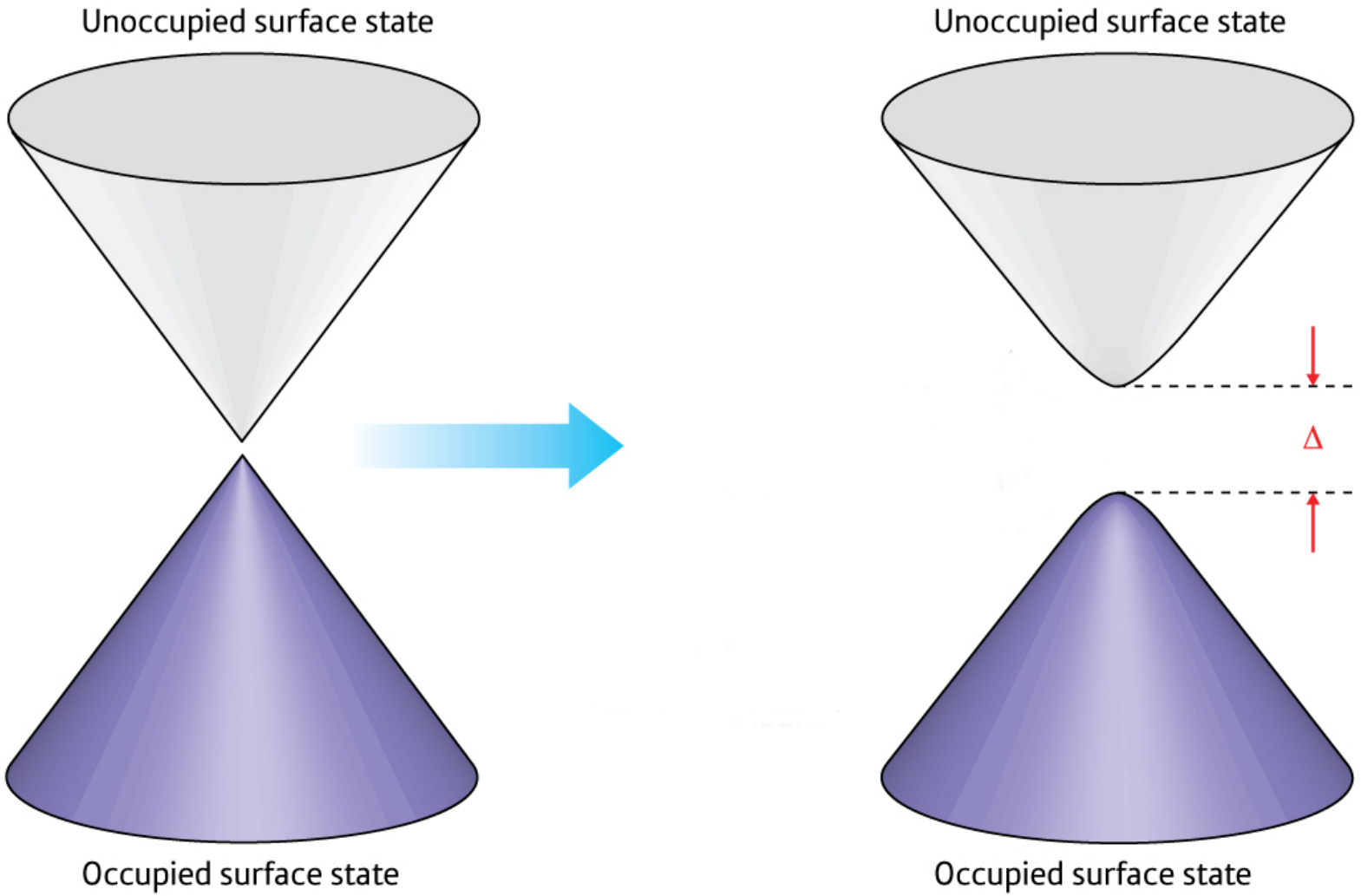
Effective theory

- $N = 2$ Massless Dirac fermions
- Fermi velocity is $v_f \ll c$
- Anisotropy in Fermi velocity $v_{\|} \neq v_{\perp}$
- Electromagnetic interaction
- Effective charge is $\alpha_F = \frac{\alpha}{\epsilon v_F} \sim 1$, $\alpha = \frac{1}{137}$

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

Semimetal - Insulator transition

At large enough α gapped phase?



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

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

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

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

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:

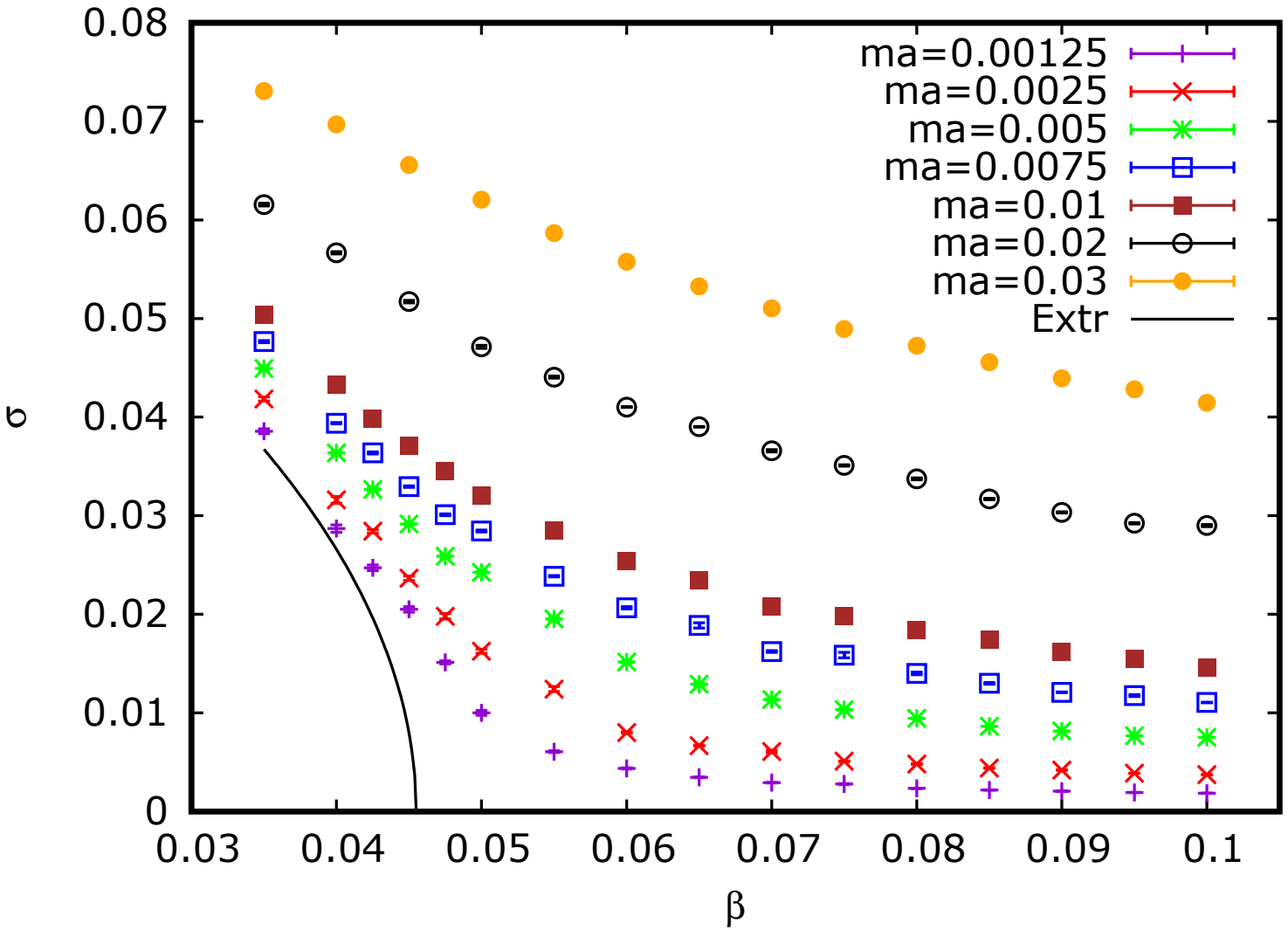
$$\chi = \frac{\partial \sigma}{\partial m} = \frac{1}{V}(\langle \mathrm{tr}^2\, D^{-1} \rangle - \langle \mathrm{tr}\, D^{-2} \rangle - \langle \mathrm{tr}\, D^{-1} \rangle^2)$$

- Logarithmic derivative:

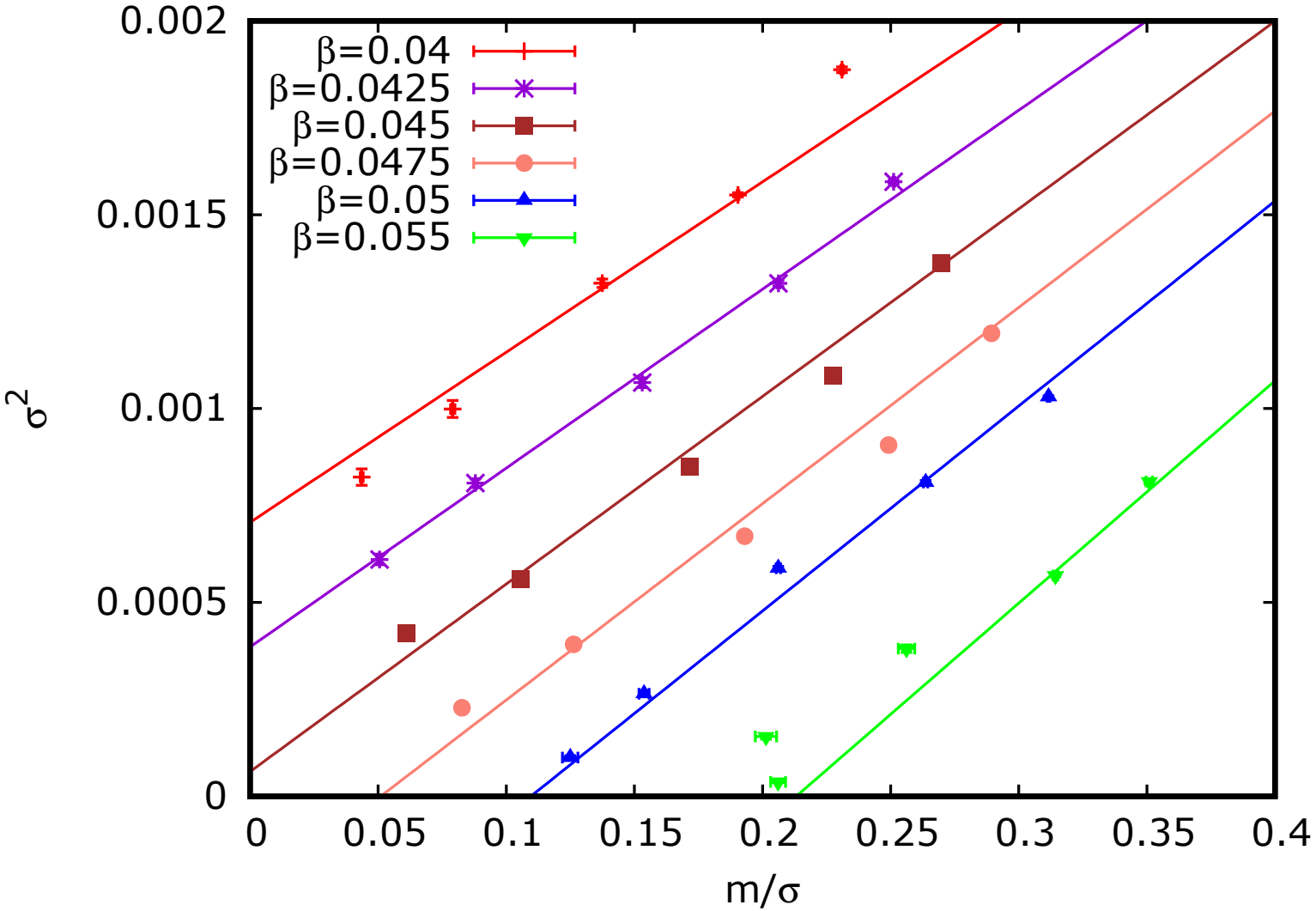
$$R = \frac{\partial \log \sigma}{\partial \log m} = \frac{m}{\sigma}\chi$$

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

$\xi = 1$. Condensate



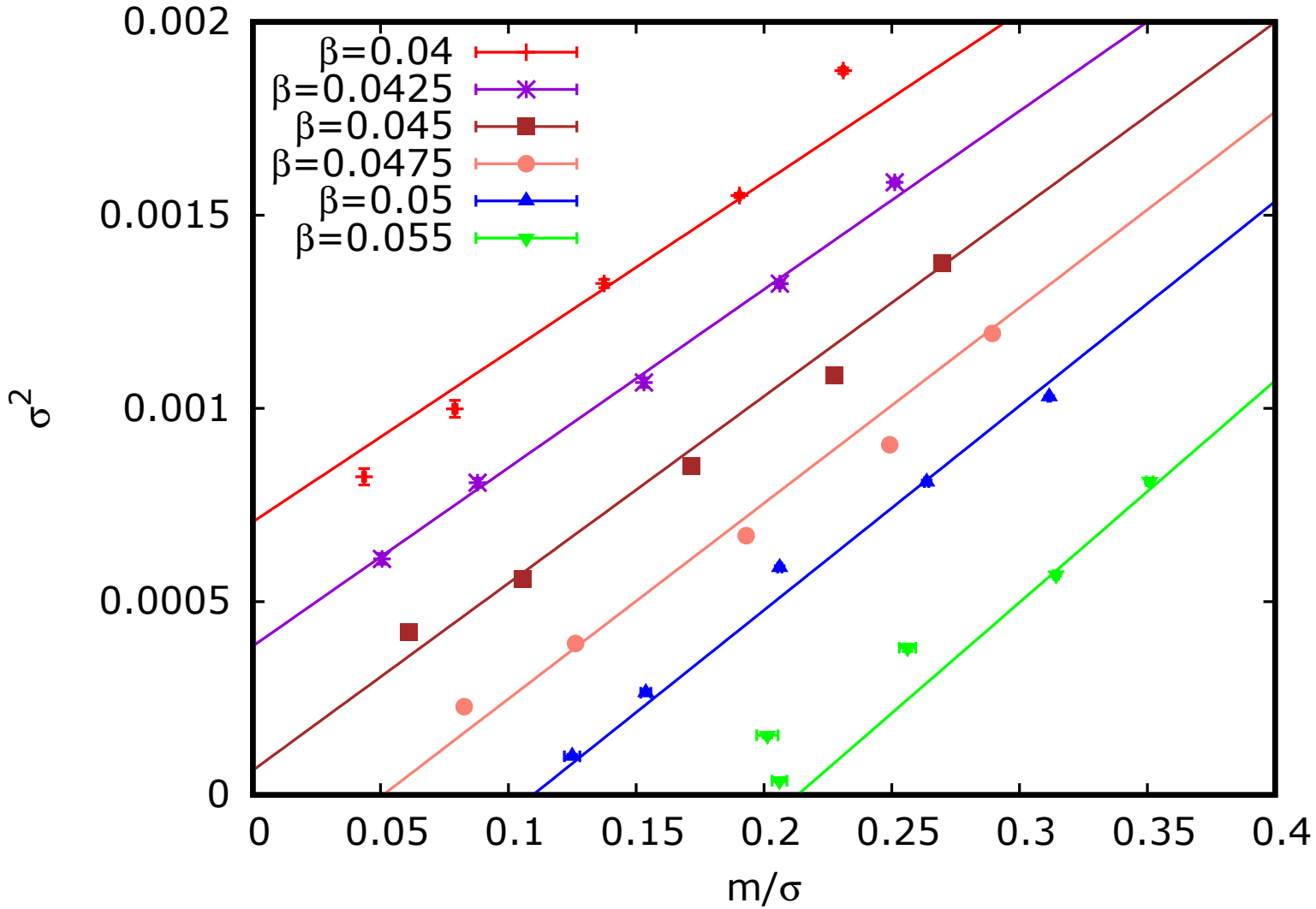
$\xi = 1$. Fisher plot



Equation of State (motivated by QED):

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

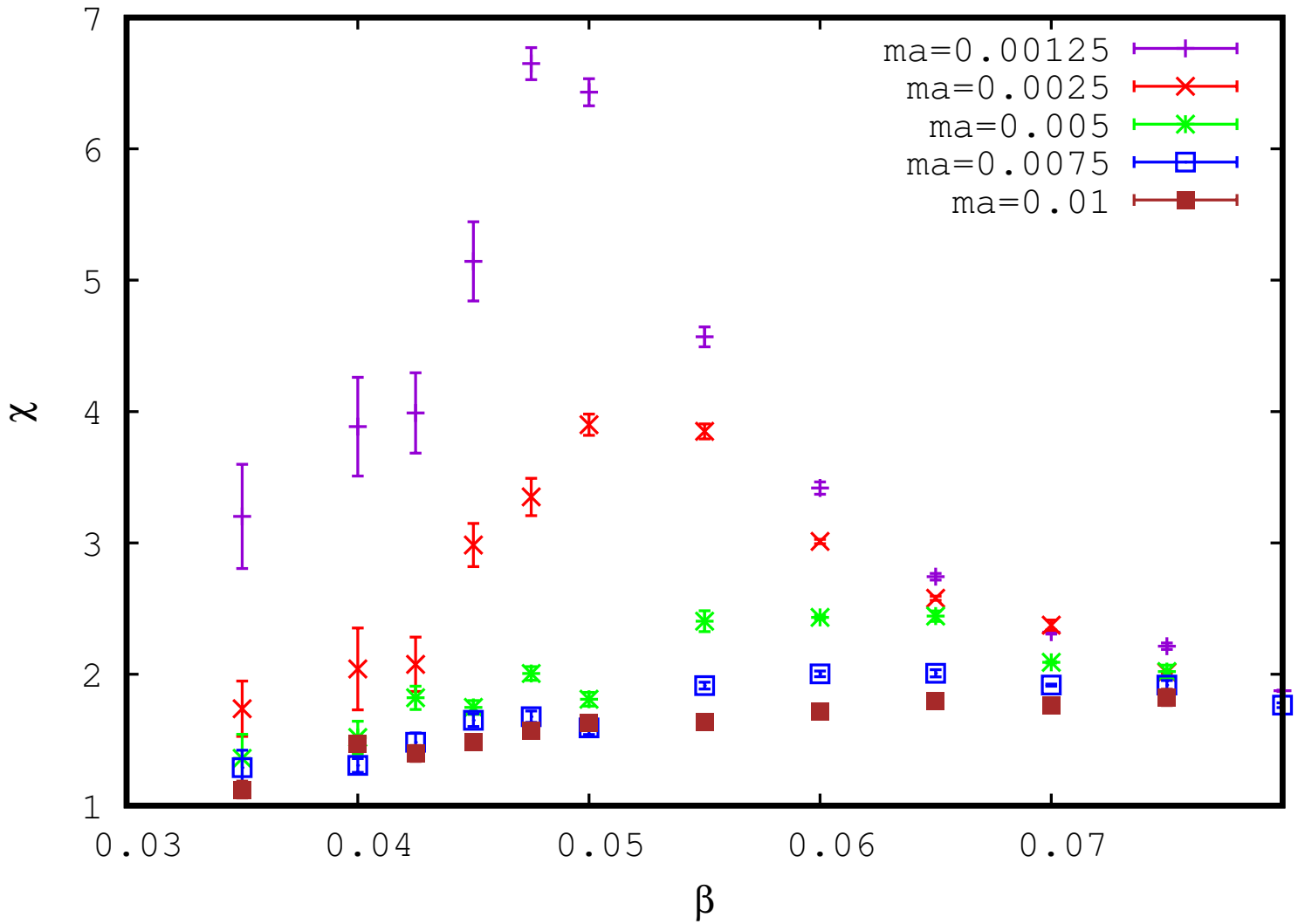
$\xi = 1$. Fisher plot



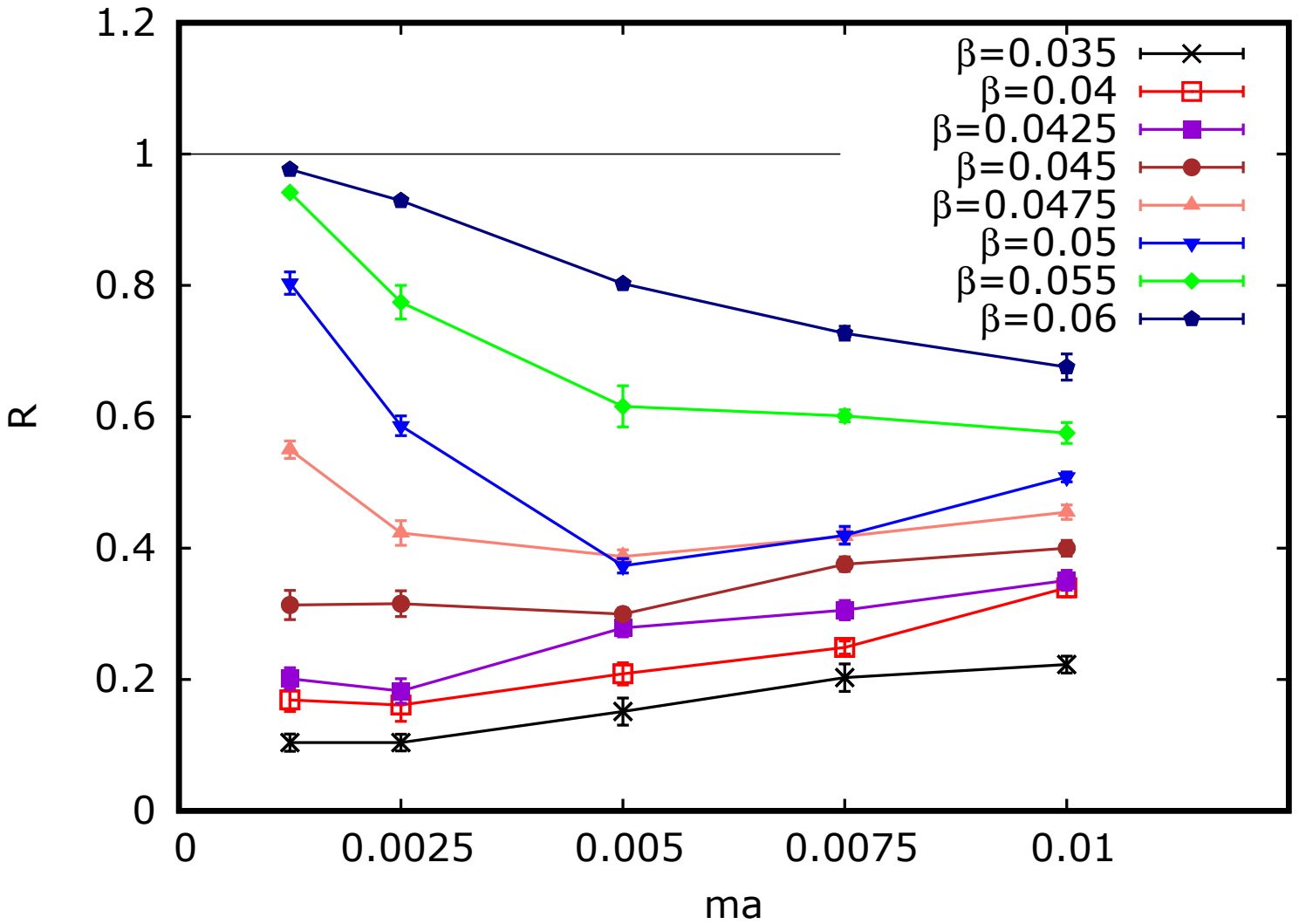
$\beta_c \sim 0.045 \rightarrow \alpha_c \sim 1.76$

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

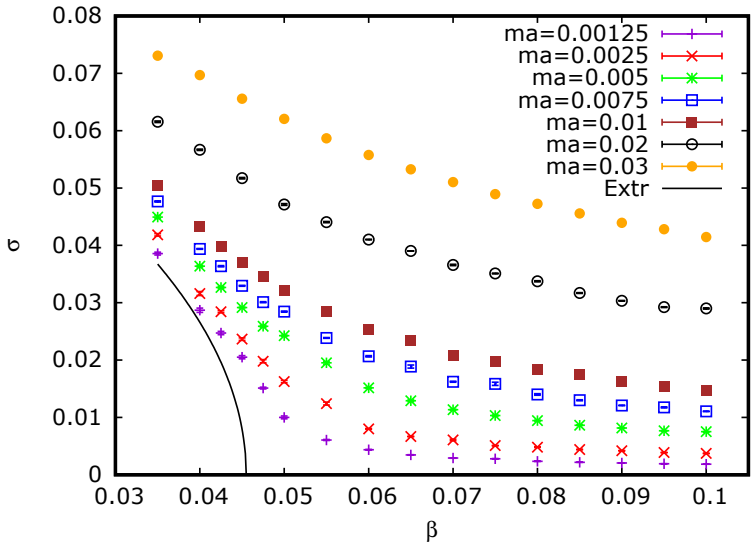
$\xi = 1$. Susceptibilities

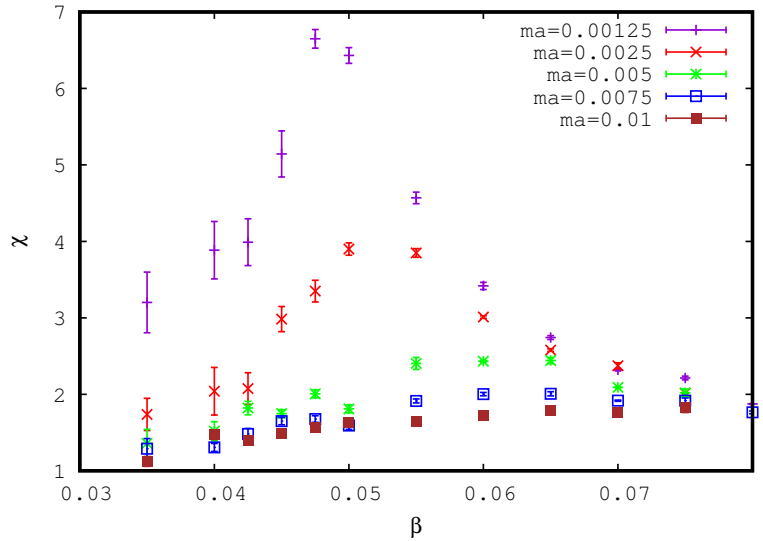


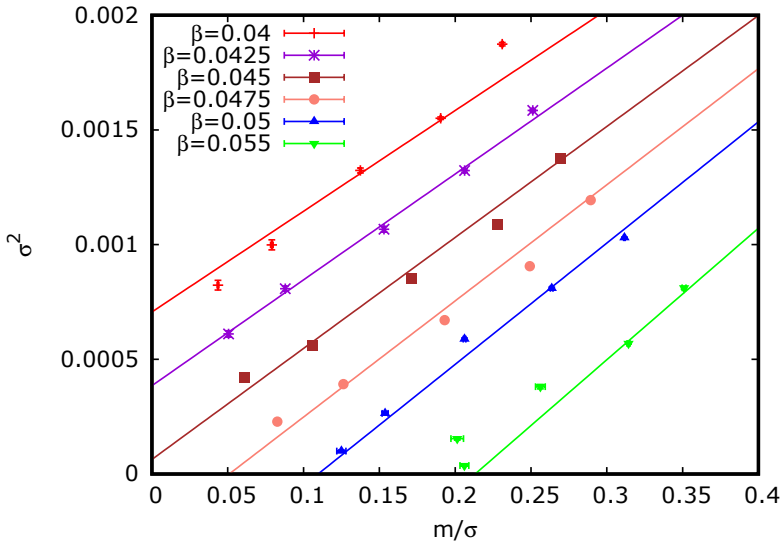
$\xi = 1$. Logarithmic derivative

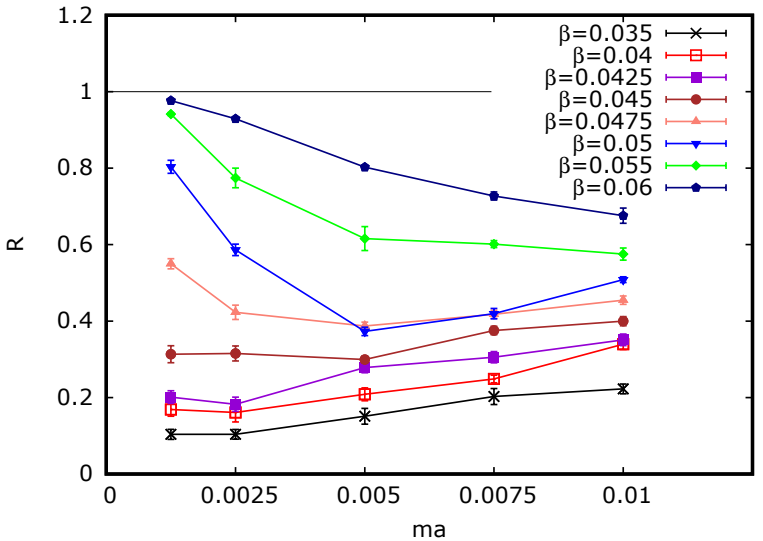


$\xi = 1$









$\beta_c \sim 0.045 \rightarrow \alpha_c \sim 1.76$

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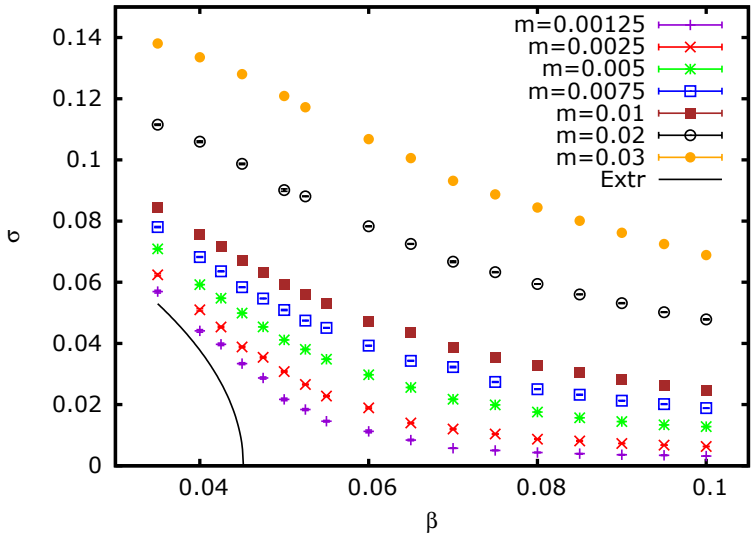
$\xi = 0.5$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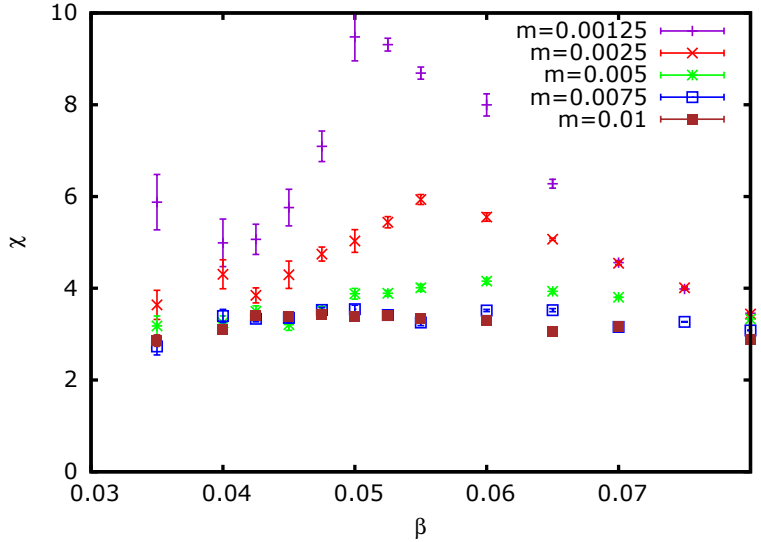
m=0.0025
m=0.005
m=0.0075
m=0.01
m=0.02
m=0.03
Extr
σ
β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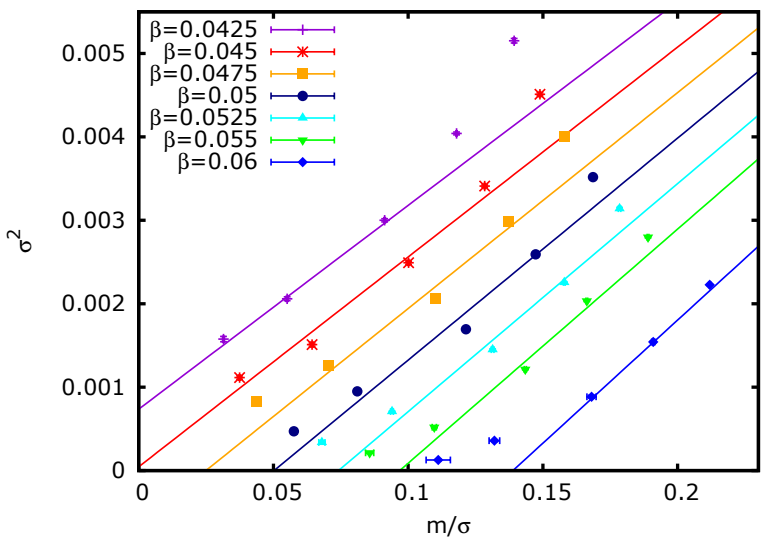
m=0.0025
m=0.005
m=0.0075
m=0.01
χ
β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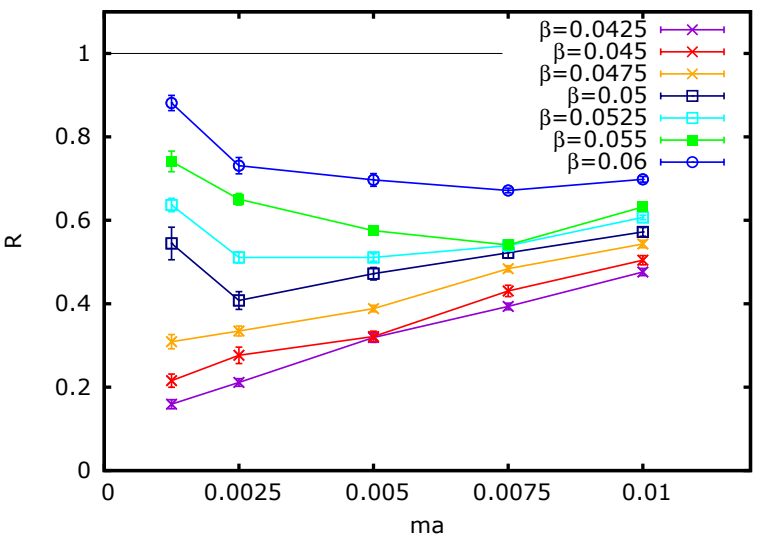
β=0.045
β=0.0475
β=0.05
β=0.0525
β=0.055
β=0.06
σ²
m/σ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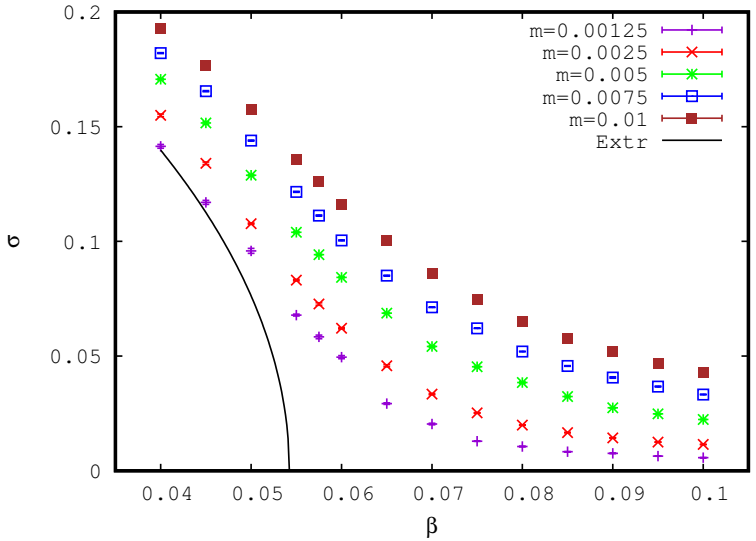
β=0.045
β=0.0475
β=0.05
β=0.0525
β=0.055
β=0.06
R
ma

$\xi = 0.2$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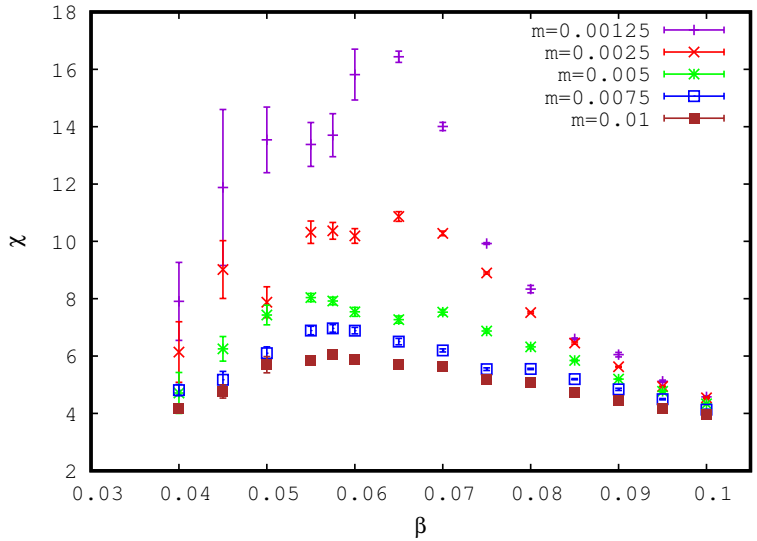
m=0.0025
m=0.005
m=0.0075
m=0.01
Extr
σ
β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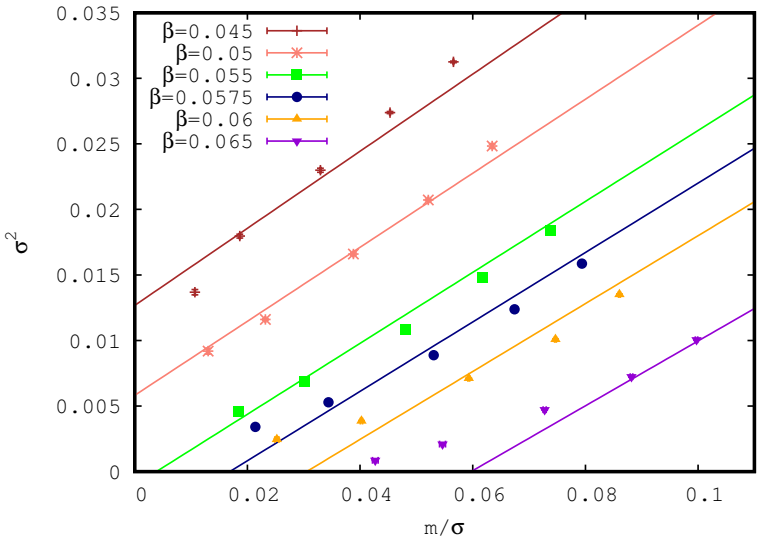
m=0.0025
m=0.005
m=0.0075
m=0.01
χ
β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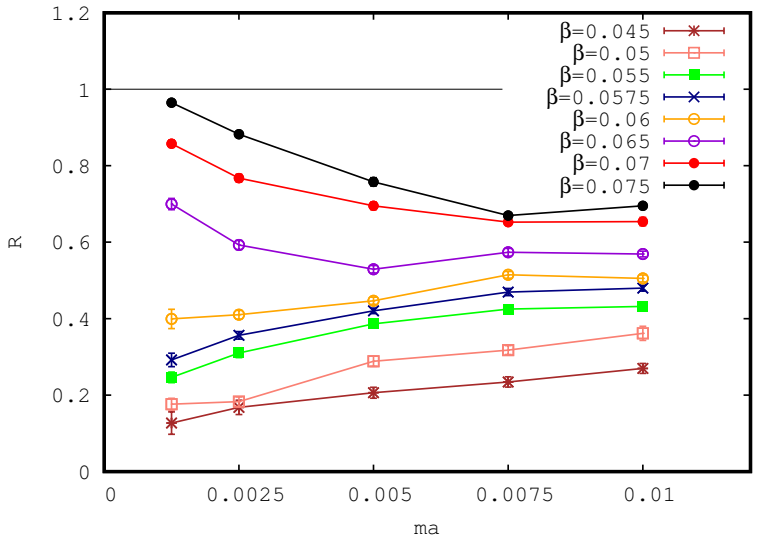
β=0.05
β=0.055
β=0.0575
β=0.06
β=0.065
σ²
m/σ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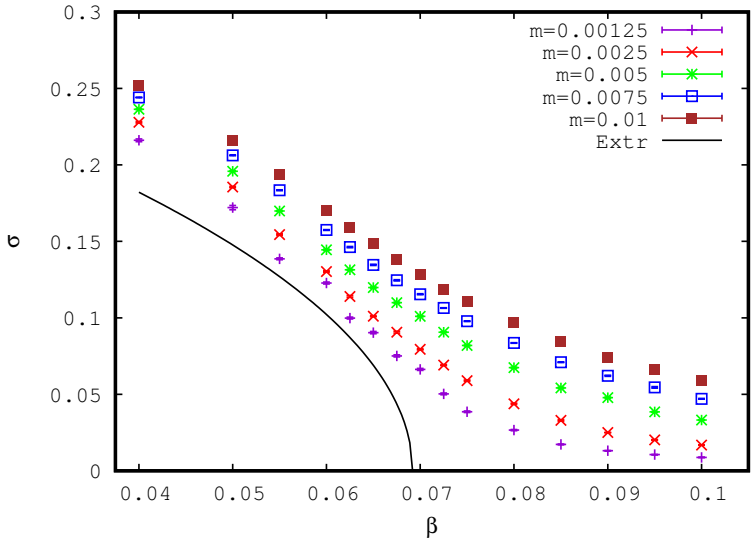
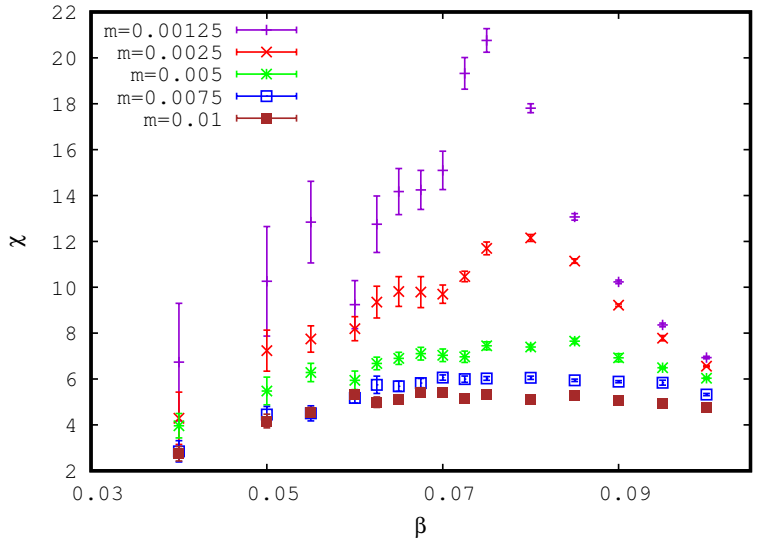
β=0.05
β=0.055
β=0.0575
β=0.06
β=0.065
β=0.07
β=0.075
R
ma

$\xi = 0.1$


m=0.00125
m=0.0025
m=0.005
m=0.0075
m=0.01
Extr
σ
β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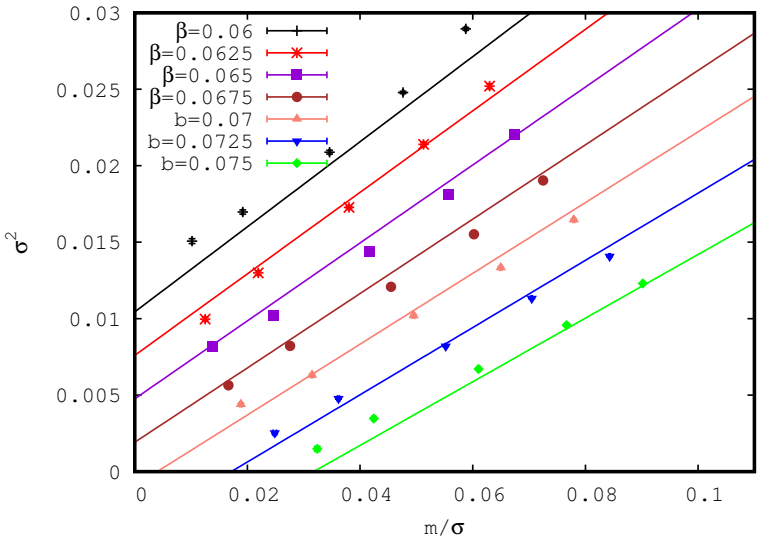
m=0.0025
m=0.005
m=0.0075
m=0.01
χ
β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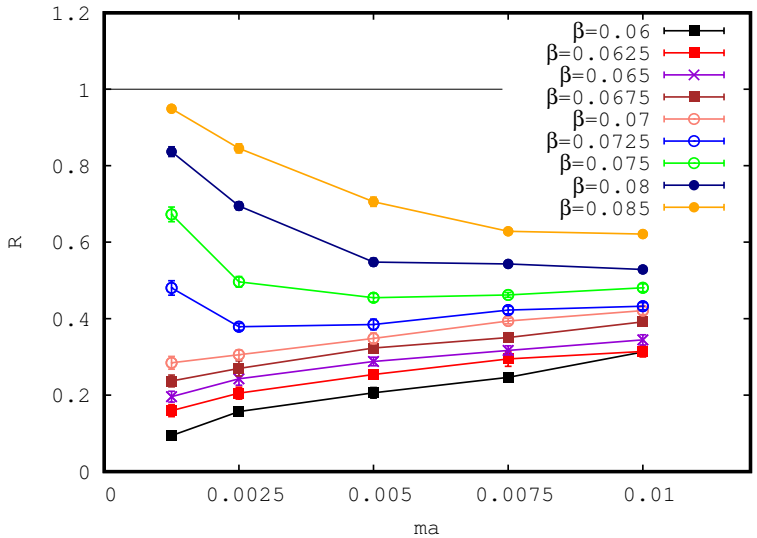
β=0.0625
β=0.065
β=0.0675
b=0.07
b=0.0725
b=0.075
σ²
m/σ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β=0.0625
β=0.065
β=0.0675
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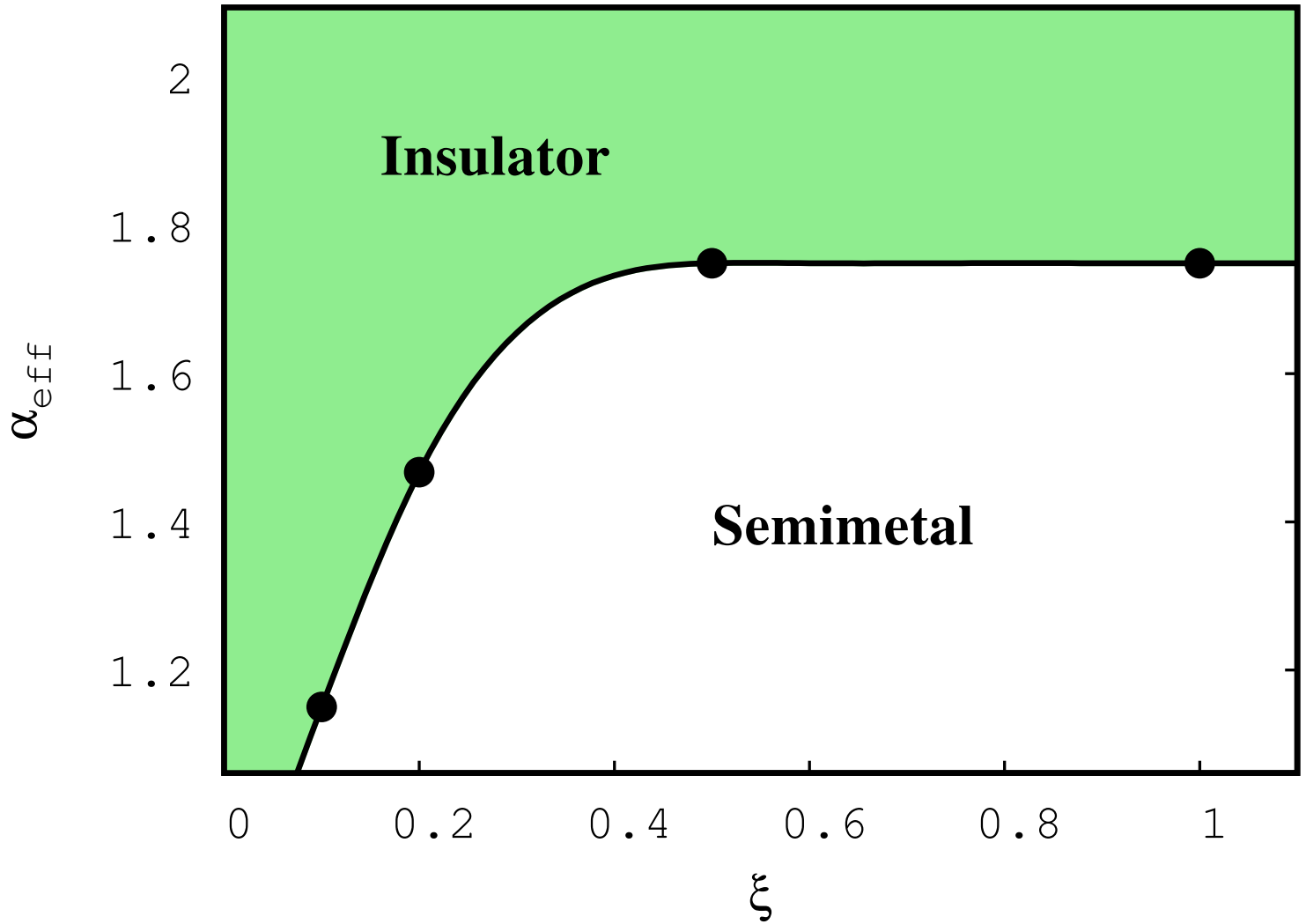
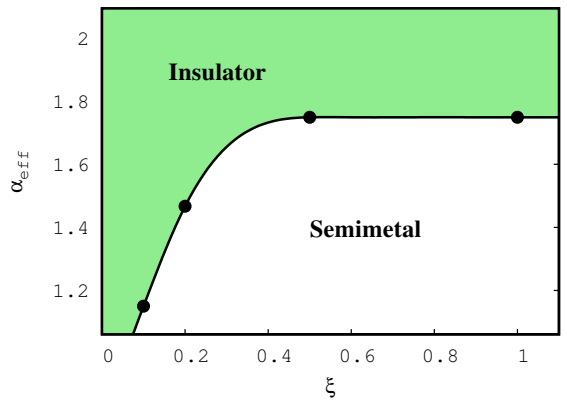
β=0.0725
β=0.075
β=0.08
β=0.085
R
ma


Insulator
Semimetal
2
1.8
1.6
1.4
1.2
α_{eff}
0
0.2
0.4
0.6
0.8
1
ξ

Conclusions

- First results of study of Dirac semimetals by means of LFT
- Semimetal-insulator transition in Dirac semimetals
- α_c decreases if we increase asymmetry
- Dimensional reduction
- Systematical uncertanties ?



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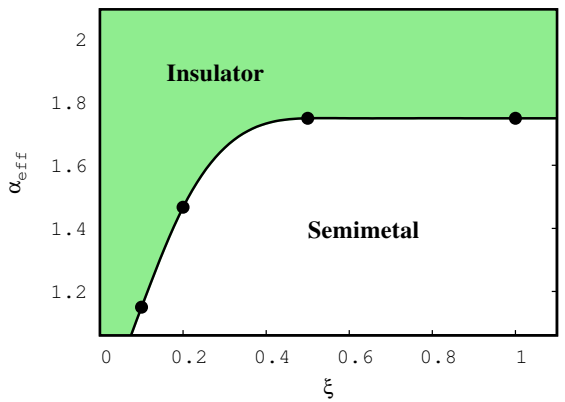

Within EFT one can study:

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