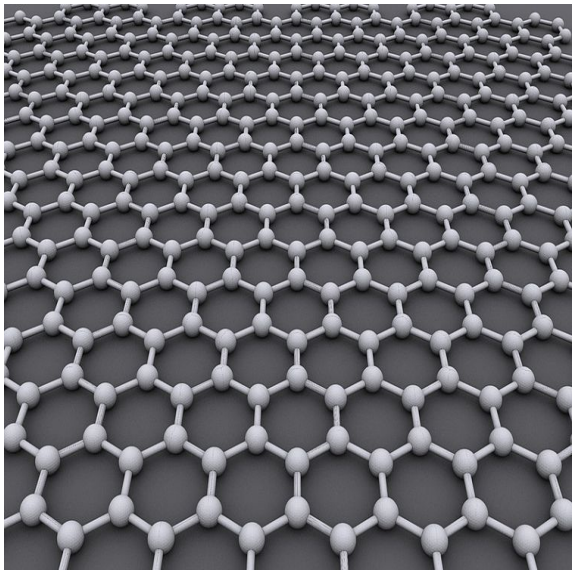
Monte-Carlo study of the semimetal-insulator phase transition in monolayer graphene with realistic inter-electron interaction potentials

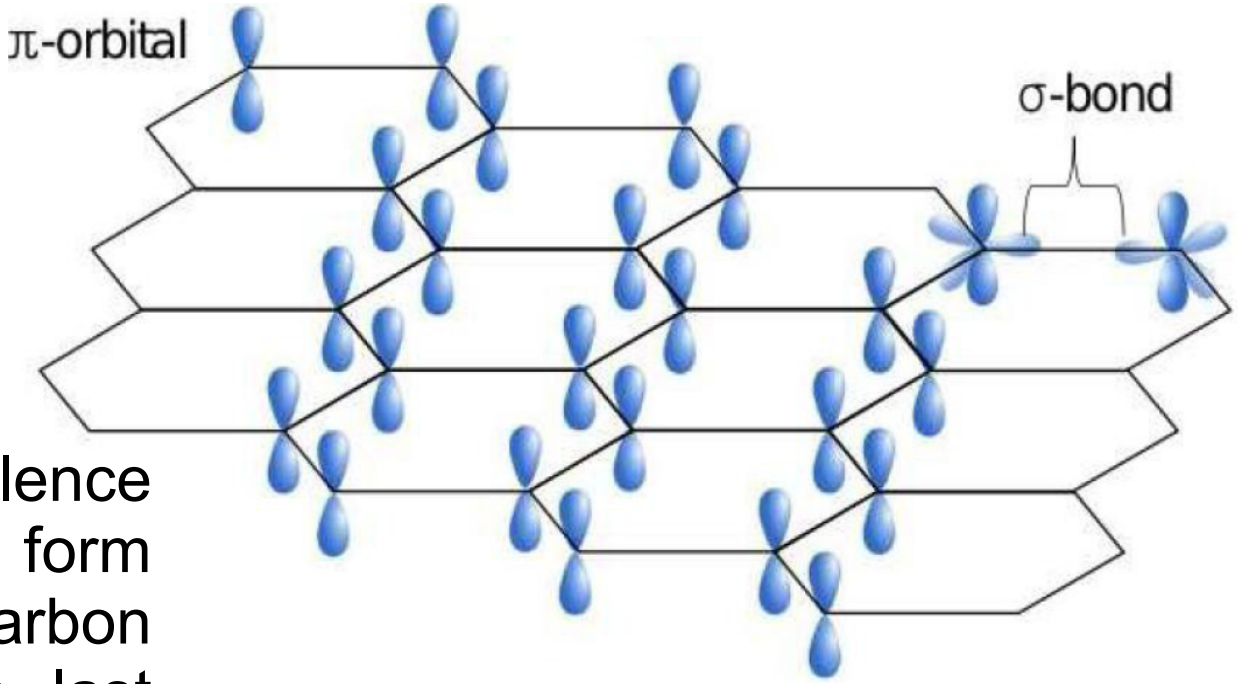
M. V. Ulybyshev, P. V. Buividovich, M. I. Katsnelson, M. I. Polikarpov

ArXiv:1304.3660, to appear in PRL

Graphene: general structure



Graphene is a two-dimensional crystal of carbon atoms, which form hexagonal lattice



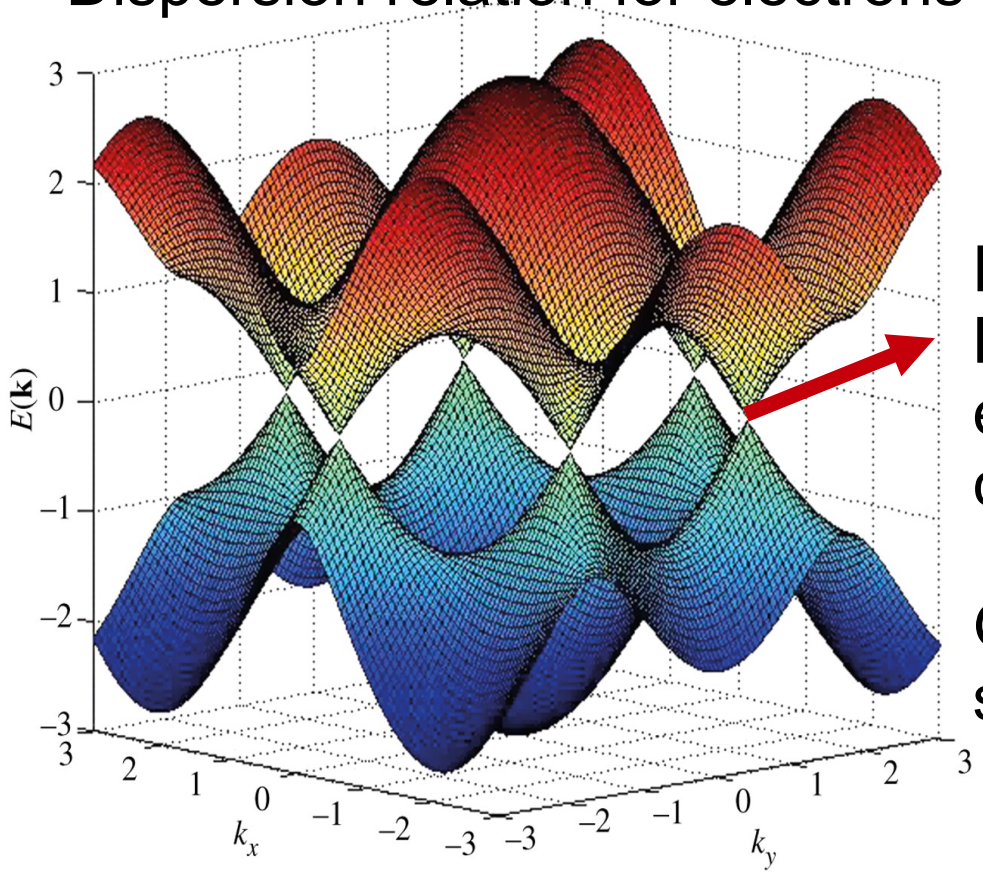
Each carbon atom has 4 valence electrons. 3 of them form chemical bonds between carbon atoms (σ-orbitals) and the last remains on π-orbital (sp^3 hybridization)

Graphene: basic electronic properties

π-orbital can be occupied by maximum 2 electrons. Graphene at «half filling» (zero chemical potential) contains only 1 electron on each π-orbital.

Therefore the π-orbitals band determines the graphene conductivity properties.

Dispersion relation for electrons on π-orbitals:



Dirac cones appear in the vertices of Brilloine zone. Low-energy electronic excitaions are 2 flavors of 4-component massless Dirac fermions.

Graphene is a semi-metal: fermi surface is reduced to «fermi points»

Graphene: Coulomb interaction

Low -energy graphene effective field model:

$$S = -\int F_{\mu\nu}F^{\mu\nu}d^3xdt + \sum_{a=1,2}\left(\int \overline{\psi_a}(i\partial_0 - eA_0)\gamma^0\psi_a d^2xdt + \int \overline{\psi_a}(i\partial_k - eA_k)\gamma^k\psi_a v_F d^2xdt\right)$$

Fermi velocity v_F =1/300c plays the role of the speed of light for fermionic field.

Therefore effective coupling constants is $\alpha = 300/127 \sim 2$.

Graphene low-energy theory is electrodynamics with very strong interaction.

Another consequence of small v_F/c ratio: we can neglect effects of retardation and consider only A_0 component of elecromagnetic field.

We can work with instantaneous Coulomb interaction, neglecting magnetic field.

Influence of Coulomb interaction on graphene conductivity

We can control the strength of the Coulomb interaction in experiment by placing graphene on a substrate or inside a media with dielectric permittivity ε. In the case of substrate the effective coupling constants varies as

$$\alpha_\varepsilon = 2\alpha/(\varepsilon+1)$$

Graphene is a conductor in the absence of Coulomb interaction. But if we turn on the interaction, the phase transition to insulator phase can appear at a certain interaction strength (e. g. at a certain dielectric permittivity of the substrate)

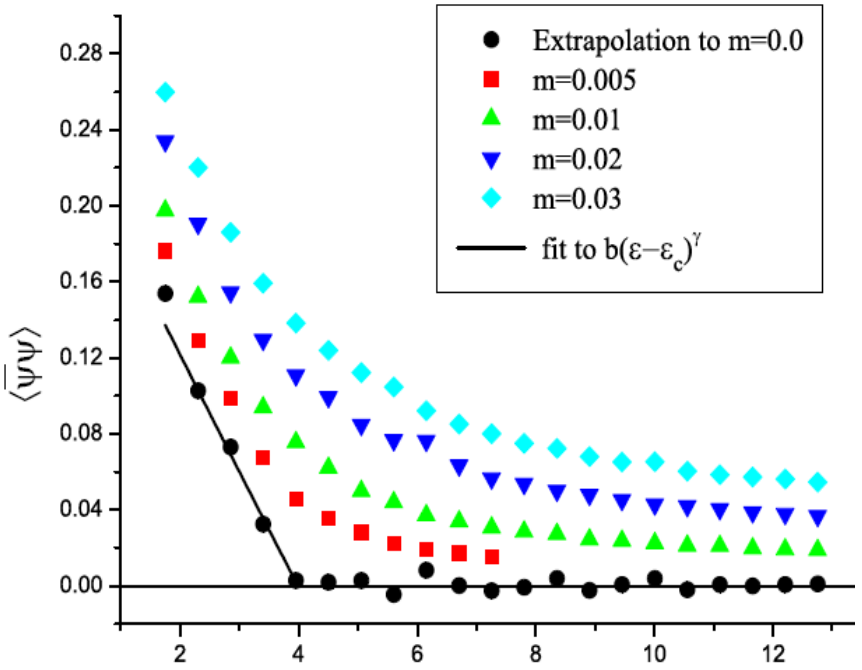
Possible generation of chiral condensate $\bar{\psi}\psi$ at some value of ε.

Influence of Coulomb interaction on graphene conductivity

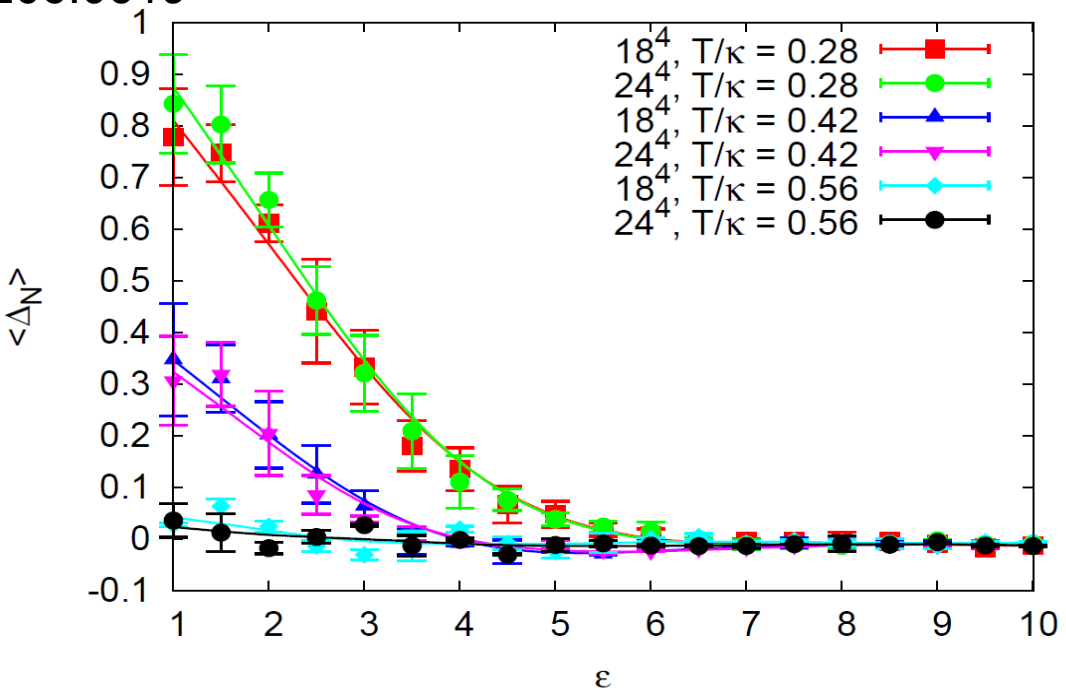
Many theoretical papers and lattice simulations predicted phase transition at ε=4.

Lattice calculations of condensate:

Joaquín E. Drut, Timo A. Lähde, arXiv:0807.0834,
P. V. Buividovich et. al., arXiv:1204.0921,
M. I. Polikarpov, P. V. Buividovich, arXiv:1206.0619

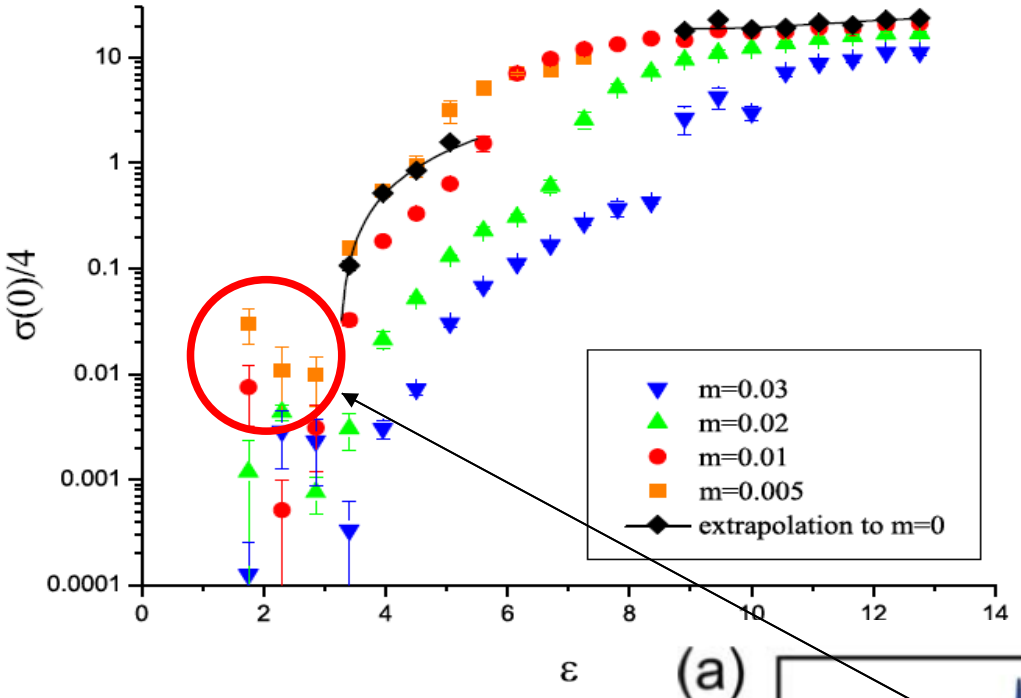


Effective field model, staggered fermions



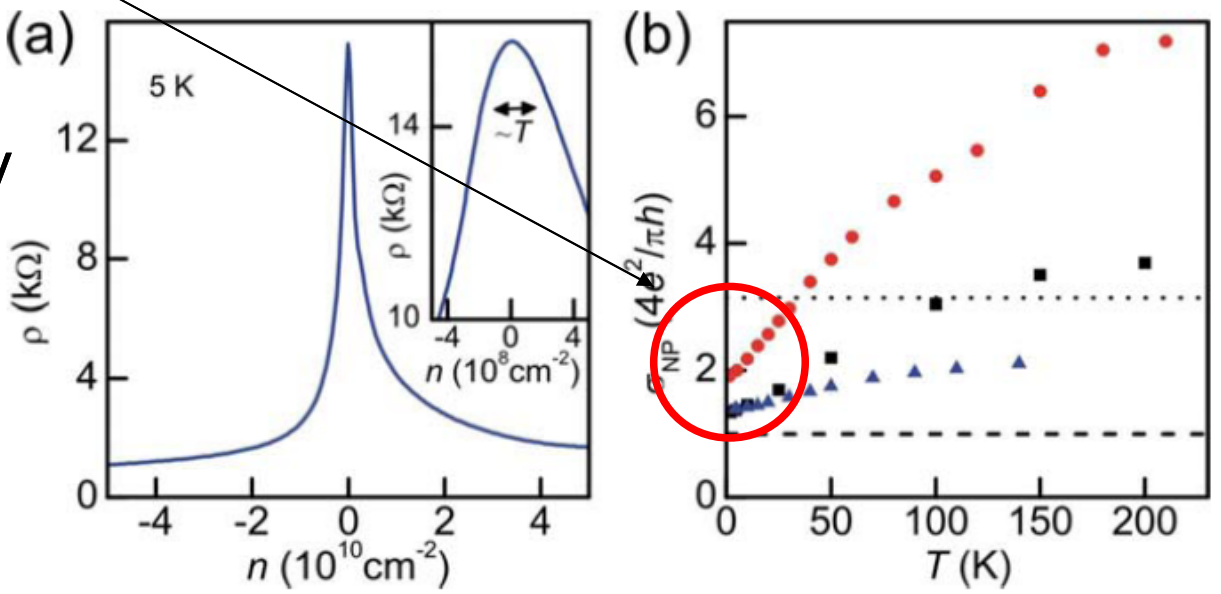
Gauge field on hexagonal lattice

Graphene conductivity: theory vs experiment



Lattice simulations, phase transition at $\varepsilon=4$

Experiment, A. S. Mayorov et. al., arXiv:1206.3848
No evidence of phase transition



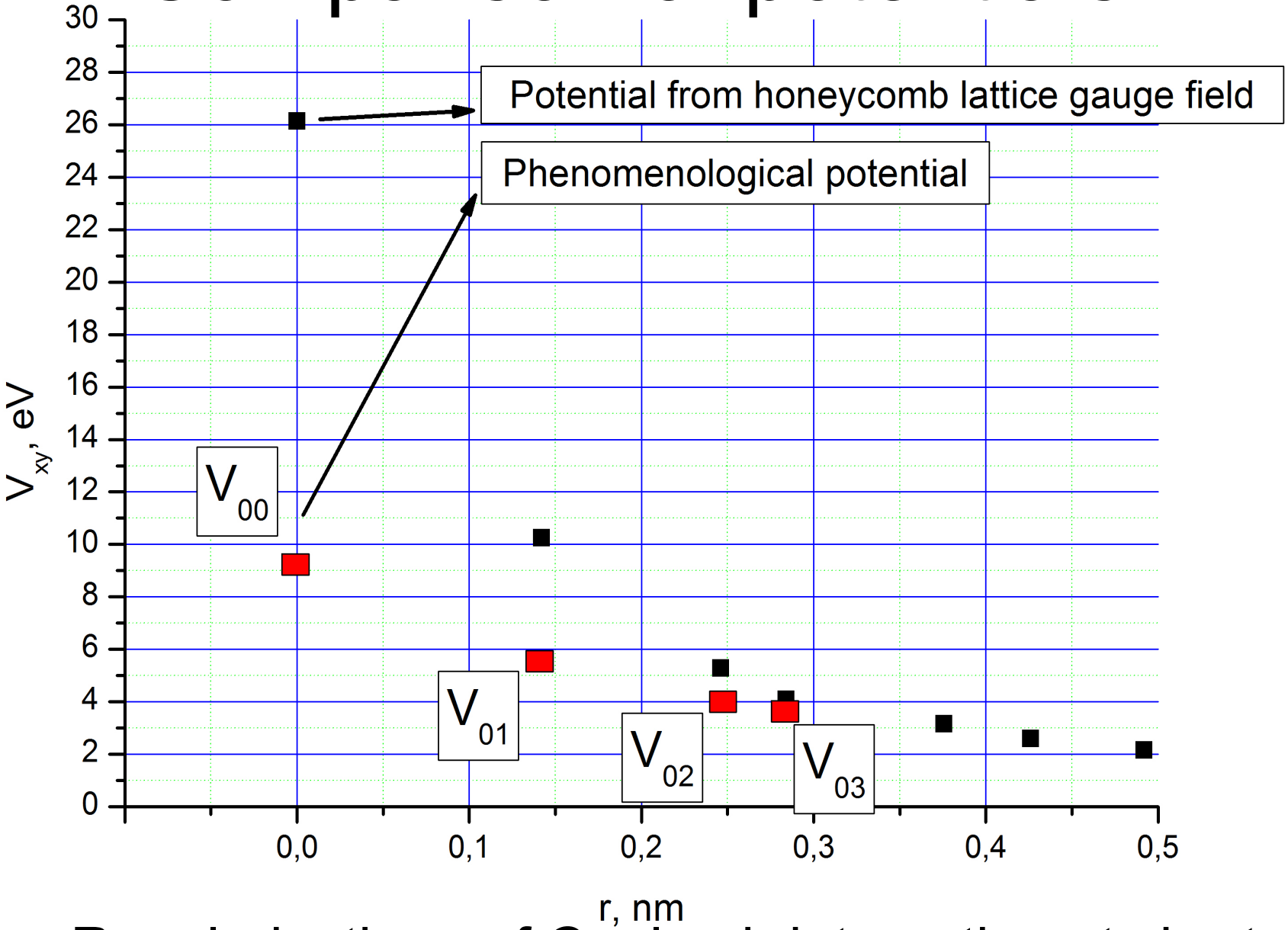
Coulomb interaction at short distances

Electron-electron interaction potentials are in fact free phenomenological parameters of the theory, because they are under strong influence of additional factors (sigma-orbitals, edges, etc.)

We are interested especially in short-range interactions, because corrections at distances comparable to the lattice step seems to be the largest ones.

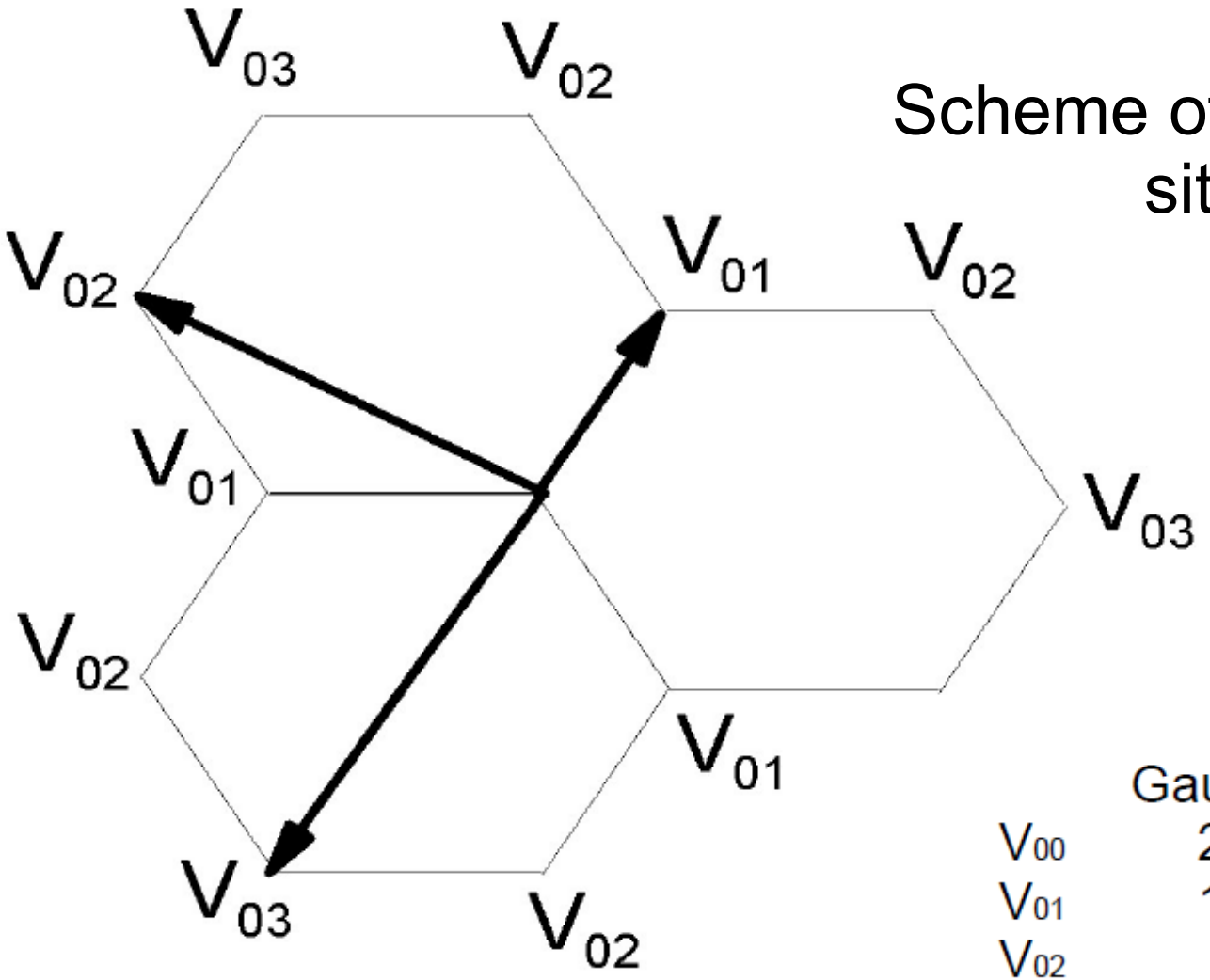
We used potentials, calculated in the paper Wehling et.al. (arXiv:1101.4007). The calculation was performed taking into account screening from σ- orbitals.

Comparison of potentials



«Regularization» of Coulomb interaction at short distances

Comparison of potentials



Scheme of neighbour sites

	Gauge field	Phenomenology
V_{00}	26.2 eV	9.3 eV
V_{01}	10.2 eV	5.5 eV
V_{02}	5.3 eV	4.1 eV
V_{03}	4.1 eV	3.6 eV

Basic definitions of the model

In order to introduce inter-electron potentials as a free parameters we should use Hubbard-Stratonovich transformation and Hubbard field instead of gauge field.

We start from tight binding hamiltonian:

$$\hat{H}_{tb} = -\kappa \sum_{<x,y>,s} \left(\hat{a}^{+}_{y,s} \hat{a}_{x,s} + \hat{a}^{+}_{x,s} \hat{a}_{y,s} \right)$$

where

$$\kappa = 2.7eV$$

$a^{+}_{x,s}$ creates electron with the spin *s* at lattice site *x*

$$\{a^{+}_{x,s} a^{+}_{x',s'}\} = \delta_{xx'}\delta_{ss'} \qquad s = \pm 1$$

Interaction

Electric charge at site x:

$$\hat{q}_x = \hat{a}^+_{x,1}\hat{a}_{x,1} + \hat{a}^+_{x,-1}\hat{a}_{x,-1} - 1$$

Introduction of «electrons» and «holes»:

$$\hat{a}_x = \hat{a}_{x,1} \qquad \hat{b}_x = \begin{cases} \hat{a}^+_{x,-1}, x \in \text{sublattice } 0 \\ -\hat{a}^+_{x,-1}, x \in \text{sublattice } 1 \end{cases}$$

Interaction hamiltonian: $\hat{H}_C = \frac{1}{2}\sum_{x,y} V_{xy}\hat{q}_x\hat{q}_y$

where $\hat{q}_x = \hat{a}^+_x\hat{a}_x - \hat{b}^+_x b_x$

Full hamiltonian: $\hat{H} = \hat{H}_C + \hat{H}_{tb}$

Tight-binding hamiltonian in terms of «electrons» and «holes»: $\hat{H}_{tb} = -\kappa \sum_{<x,y>} \left(\hat{a}^+_y\hat{a}_x + \hat{b}^+_y\hat{b}_x + h.c.\right)$

Converting to a form convenient for Monte-Carlo calclulations

Partition function:

$$\mathrm{Tr}(e^{-(H_{tb}+H_C)\beta}) \approx \mathrm{Tr}(e^{-H_{tb}\delta} I e^{-H_C\delta} I e^{-H_{tb}\delta} I e^{-H_C\delta} I .....)$$

Introduction of fermionic coherent states:

$$|\psi, \eta\rangle = e^{-\sum_x \psi_x a_x^+ + \eta_x b_x^+} |\Omega\rangle$$

Using the following relations:

$$\int d\psi d\eta d\psi^+ d\eta^+ e^{-\sum_x \psi_x^+ \psi_x} |\psi, \eta\rangle\langle\psi^+, \eta^+| = I$$

$$\langle\psi|F(a^+, a)|\psi\rangle = F(\psi^+, \psi) e^{\psi^+\psi}$$

$$\langle\eta| \exp\left(\sum_{i,j} A_{ij} \hat{\psi}_i^\dagger \hat{\psi}_j\right) |\eta'\rangle = \exp\left(\sum_{i,j} \left(e^A\right)_{ij} \bar{\eta}_i \, \eta'_j\right)$$

and Hubbard-Stratonovich transformation:

$$\int \prod d\varphi_x \exp\left(-\frac{1}{2}\sum_{x,y}\varphi_x V^{-1}_{x,y}\varphi_y - i\sum_x \varphi_x Q_x\right) \cong \exp\left(-\frac{1}{2}\sum_{x,y} Q_x V_{x,y} Q_y\right)$$

We arrive at the following representation for partition function:

$$\mathrm{Tr}(e^{-H\beta}) = \int D\psi D\eta D\psi^+ D\eta^+ \exp\left(-\sum_{x,y,t,t'} \eta^+_{x,t} M^*_{x,y,t,t'}\eta_{y,t'} - \sum_{x,y,t,t'} \psi^+_{x,t} M_{x,y,t,t'}\psi_{y,t'} - S_{Hubbard}\right)$$

Where action for Hubbard field is simply the quadratic form:

$$S_{Hubbard} = \frac{\delta}{2}\sum_{x,y,t} \varphi_{x,t} V^{-1}_{x,y}\varphi_{y,t}$$

and...

Fermionic «action»

can be written as follows:

$$\sum_{x,y,t,t'} \psi^{+}_{x,t} M_{x,y,t,t'} \psi_{y,t'} = \sum_{n=0}^{N_t-1} \Bigg[\sum_{x} \psi^{+}_{x,2n}(\psi_{x,2n} - \psi_{x,2n+1}) +$$

$$+ \sum_{x} \psi^{+}_{x,2n+1}\psi_{x,2n+1} - \delta\kappa \sum_{<x,y>} \left(\psi^{+}_{x,2n}\psi_{y,2n+1} + \psi^{+}_{y,2n}\psi_{x,2n+1}\right) +$$

$$+ m\delta \sum_{1st\ subLat} \psi^{+}_{x,2n}\psi_{x,2n+1} - m\delta \sum_{2d\ subLat} \psi^{+}_{x,2n}\psi_{x,2n+1} - \sum_{x} e^{-i\delta\phi_{x,2n+1}} \psi^{+}_{x,2n+1}\psi_{x,2n+2} \Bigg]$$

Two sign problems!

1) Fermion determinant

2) Quadratic form for Hubbard field.

Comparison with previous approaches

Fermionic operator in the paper of C. Rebbi et. al (arXiv:1101.531) - «non-compact» interaction with hubbard field:

$$Z = \lim_{N_t \to \infty} \int \prod_{x,t} d\psi^*_{x,t} d\psi_{x,t} d\eta^*_{x,t} d\eta_{x,t} d\phi_{x,t}$$

$$\times e^{-\sum_{x,y,t} \phi_{x,t} (V^{-1})_{x,y} \phi_{y,t} \delta/4}$$

$$\times e^{-\sum_{x,t,y,\tau} (\psi^*_{x,t} M_{x,t;,y,\tau} \psi_{y,\tau} + \eta^*_{x,t} M_{x,t;y,\tau} \eta_{y,\tau})}$$

$$\times e^{-\sum_{x,t} \imath e \phi_{x,t} (\psi^*_{x,t} \psi_{x,t} - \eta^*_{x,t} \eta_{x,t}) \delta}.$$

$$\sum_{m,n} \psi^*_m M_{m,n} \psi_n = \sum_t \Big[\sum_x \psi^*_{x,t} (\psi_{x,t+1} - \psi_{x,t})$$

$$+ e^2 V_{xx} \psi^*_{x,t} \psi_{x,t} - \kappa \sum_{\langle x,y \rangle} (\psi^*_{x,t} \psi_{y,t} + \psi^*_{y,t} \psi_{x,t})\, \delta \Big]$$

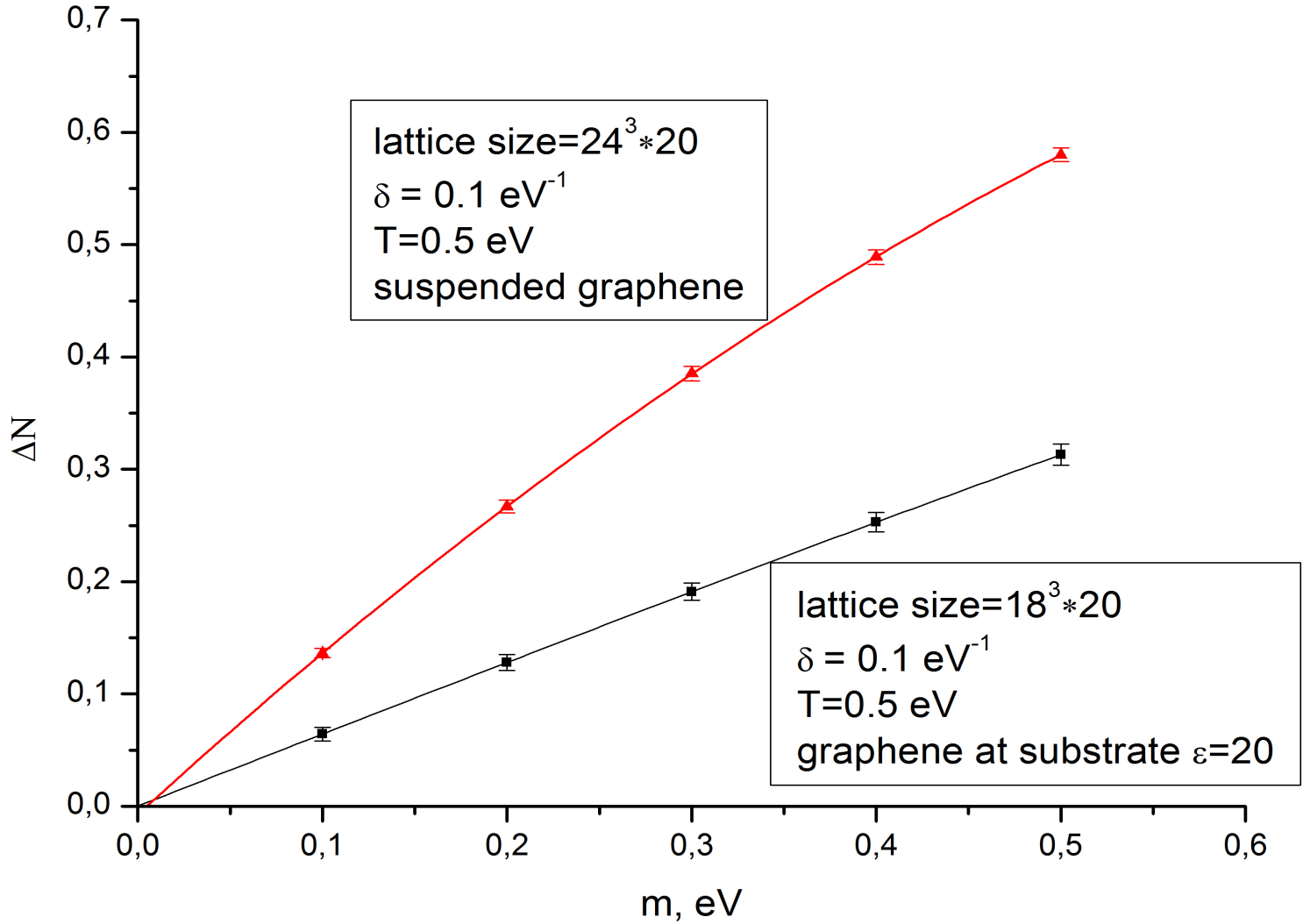
Monte-Carlo process

$$Tr(e^{-H\beta}) = \int \prod_{x,i} d\varphi_x^{(i)} \underbrace{e^{S_{Hubbard}} \det(MM^+)}_{\text{We generate configurations of Hubbard field with this probability distribution.}} =$$

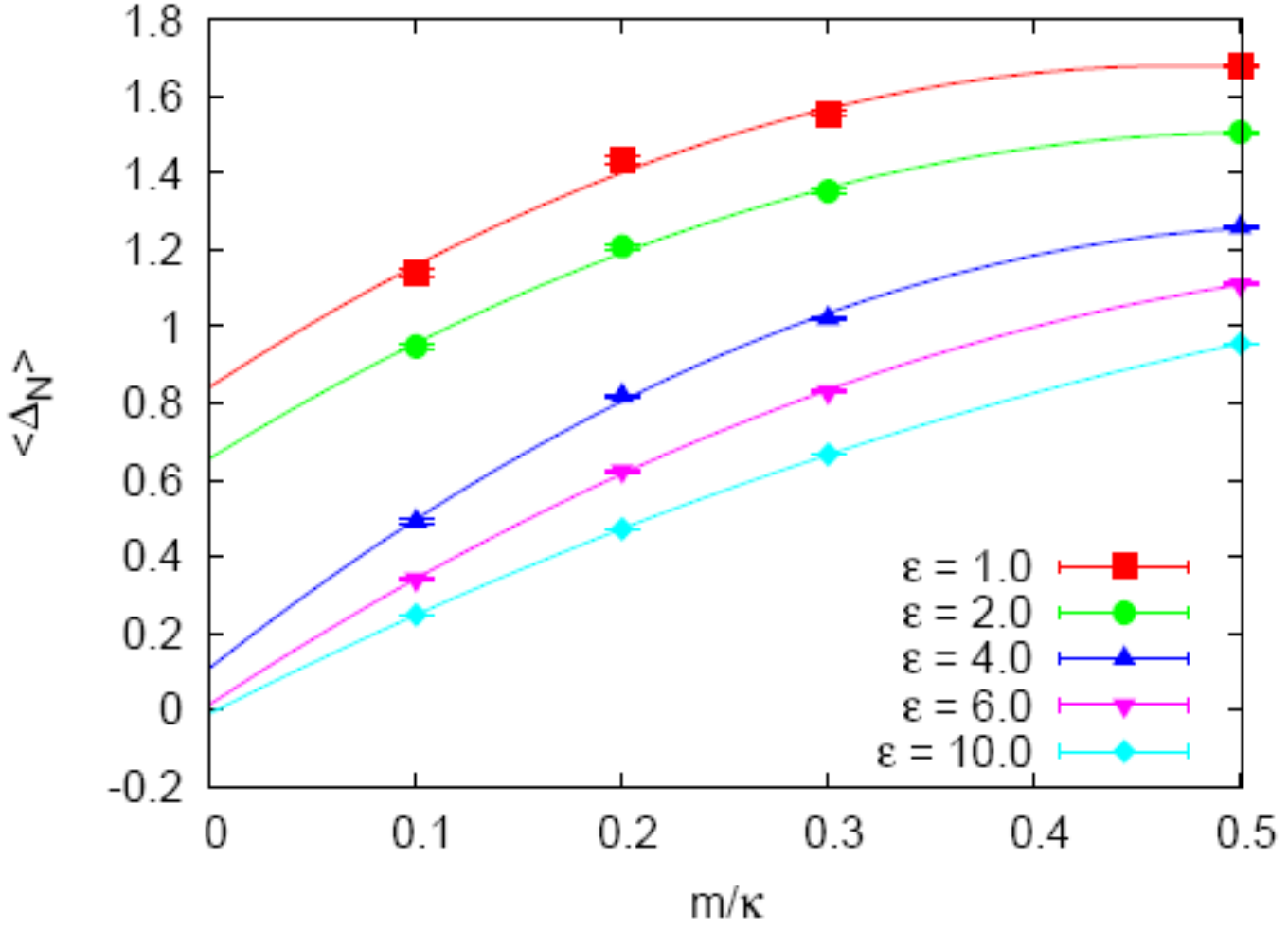
$$= \int \prod_{x,i} d\varphi_x^{(i)} \prod_{x,i} d\chi_x^{(i)*} d\chi_x^{(i)} e^{-S_{Hubbard}} e^{-\vec{\chi}^* \frac{1}{MM^+} \vec{\chi}}$$

We adopt usual Hybrid Monte Carlo algorithm to generate hubbard field configurations.

Suppression of condensate for suspended graphene — at T=0.5 eV it is still a conductor.



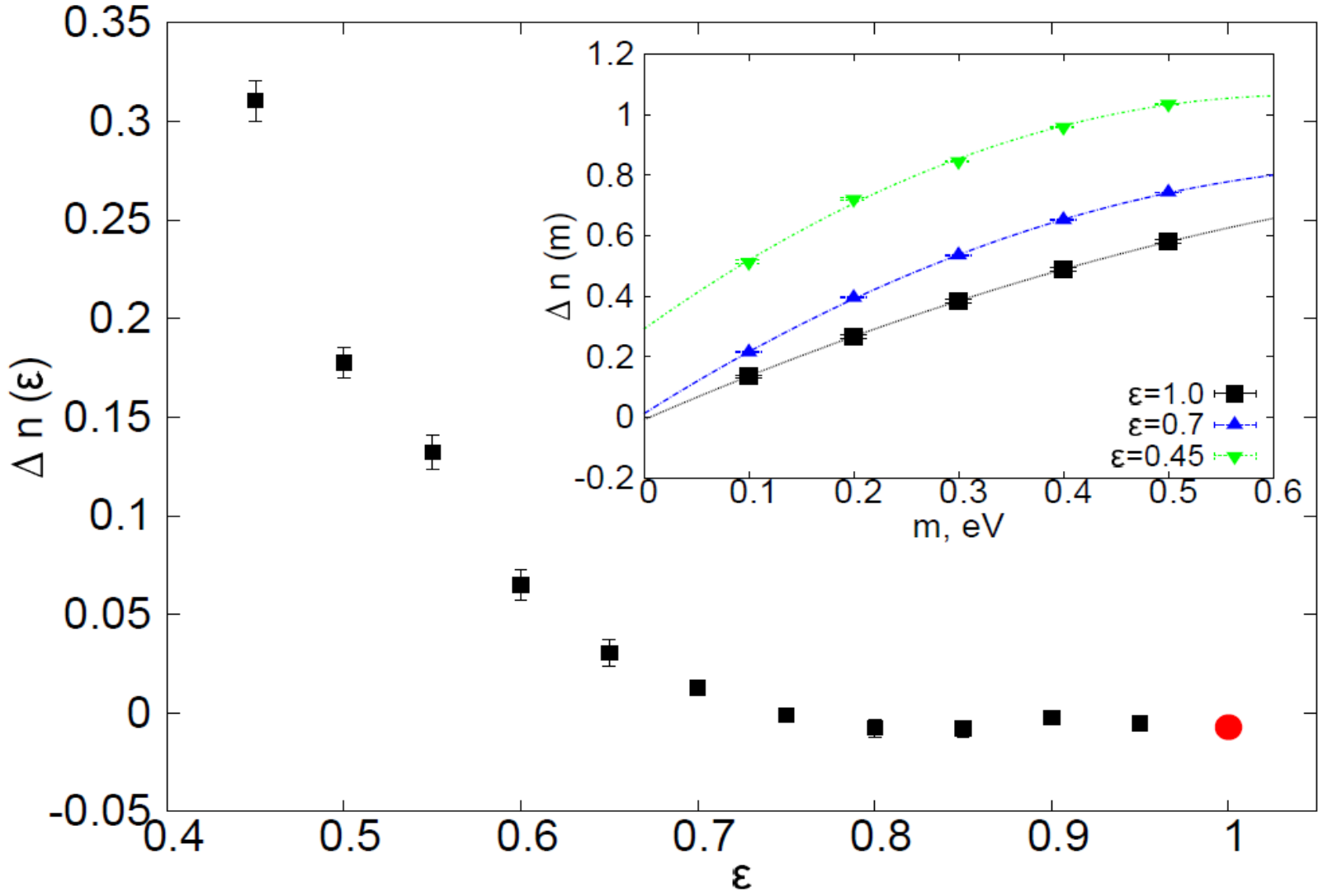
Comparison with the calculation which used gauge field on hexagonal lattice (P. V. Buividovich, M. I. Polykarpov, arXiv: 1206.0619)



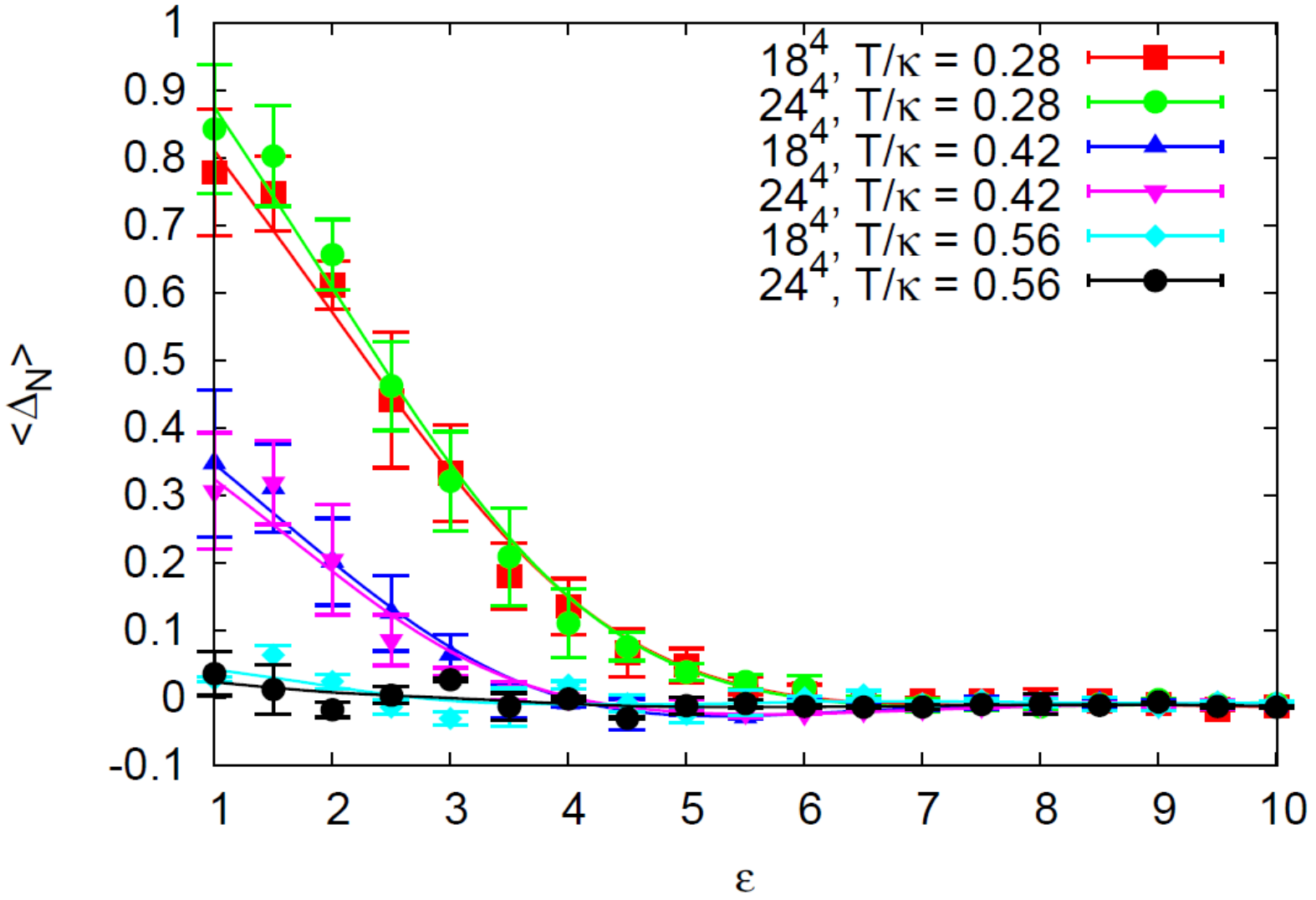
$$T/\kappa = 0.28 \quad (\kappa \Delta\tau = 0.15)$$

Phase transition appears at «unphysical» dielectric permittivity (ε<1)

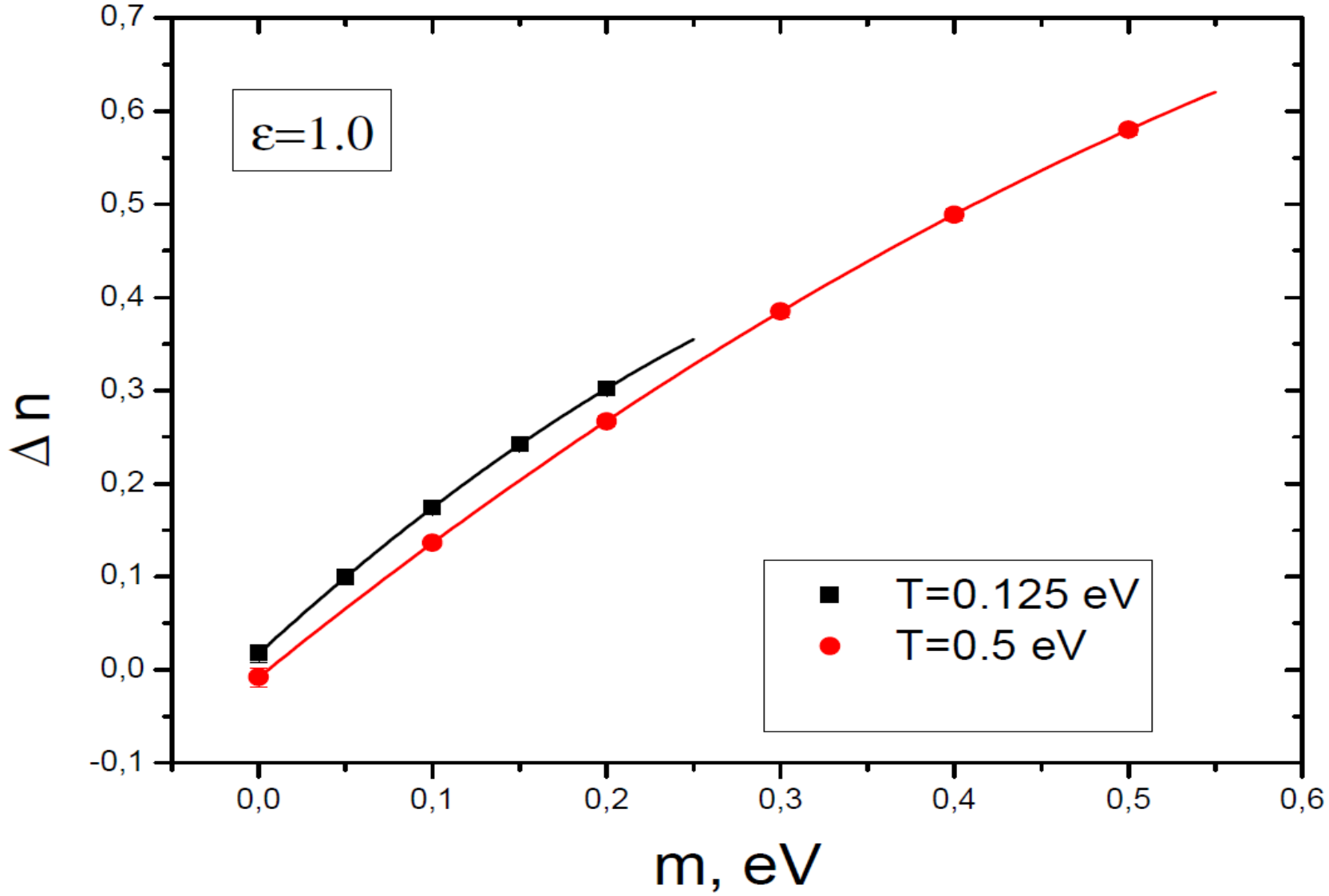
$$V_{xy} \to V_{xy}/\epsilon$$



Comparison with the calculation which used gauge field on hexagonal lattice (P. V. Buividovich, M. I. Polykarpov, arXiv: 1206.0619)



Low-temperature simulations: suspended graphene is still a conductor



Conclusions

Regularization of Coulomb potential at short distances strongly affects the conductor-insulator phase transition in graphene.

Though the suspended graphene is a conductor, the phase transition still exists at unphysical dielectric permittivity $\varepsilon \sim 0.7$.