Chiral symmetry breaking in graphene: a lattice study of excitonic and antiferromagnetic phase transitions

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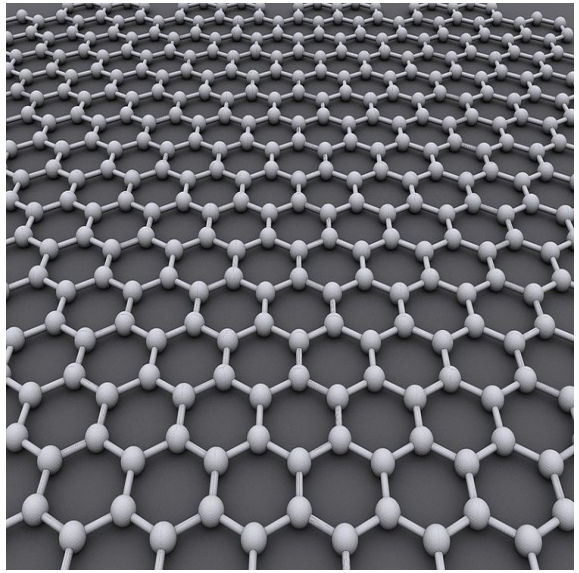
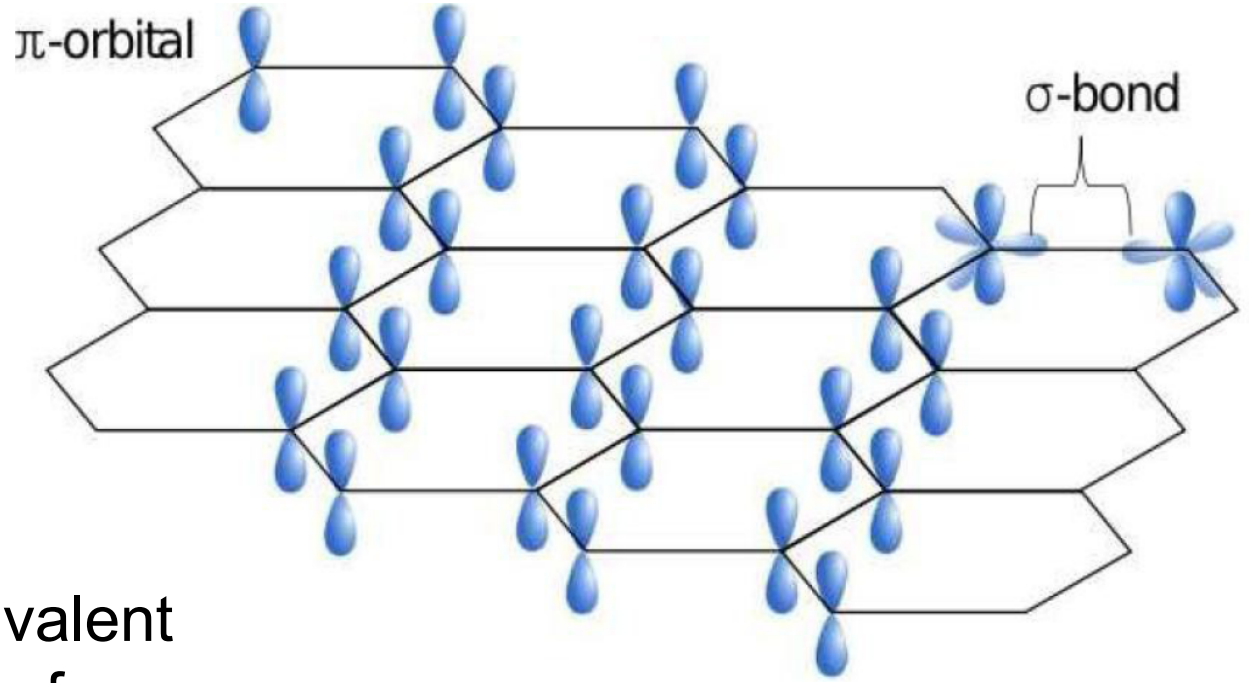
Graphene: spatial structure



Graphene is a 2-dimensional honeycomb lattice of carbon atoms:



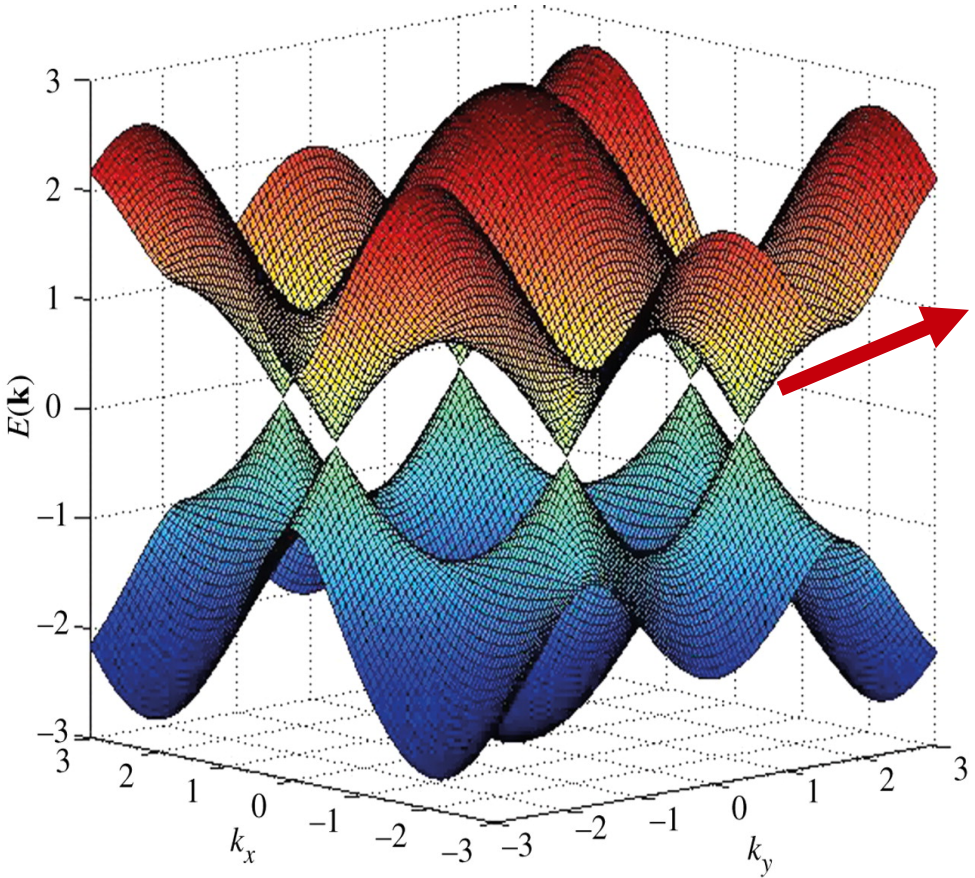
Each carbon atom has 3 valent electrons. 3 of them form chemical bonds between atoms (σ-orbitals), another one forms π-orbital (sp^3 - hybridization)

Graphene: electronic properties

There can only be a maximum of two electrons on the π-orbital. Graphen at «half-filling» (zero chemical potential): the number of electrons on π-orbitals is equal to the number of atoms.

Therefore, electrons on π-orbitals can easily move from one atom to the neighbouring one thus determine the electronic properties of graphene.

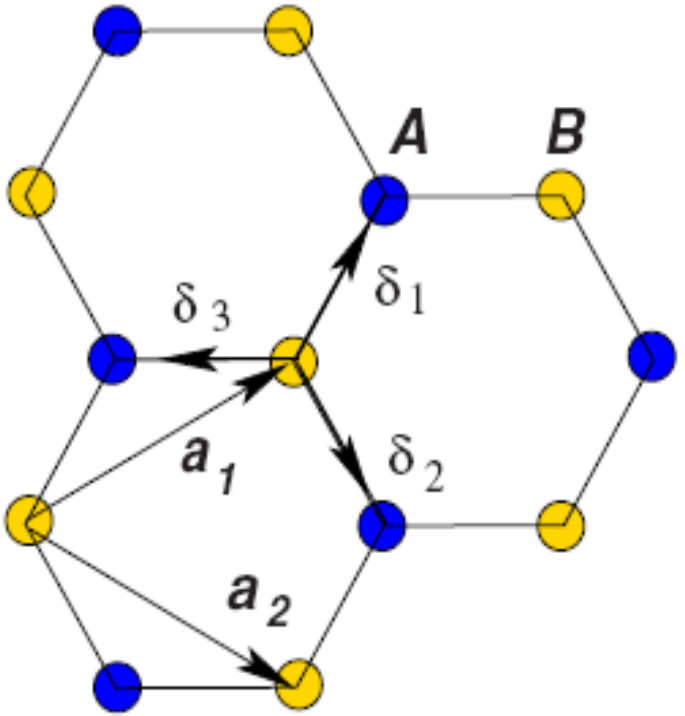
Dispersion relation:

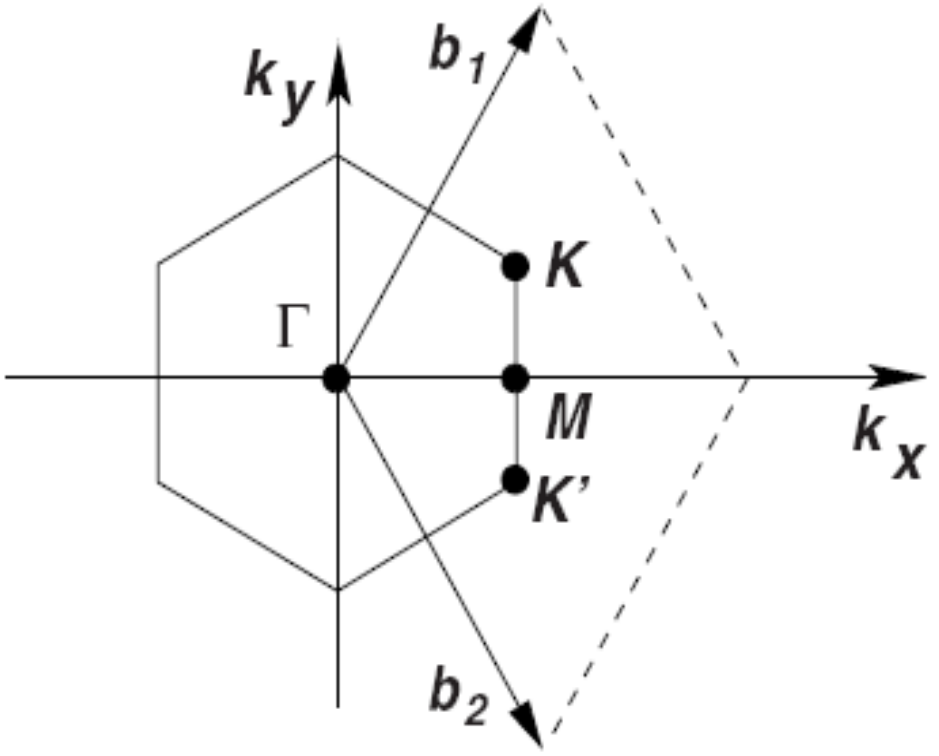


Dirac cones appear at the 2 non-equivalent points within the Brillouine zone. So, low-energy excitations can be described as 2 flavours of 4-component massless Dirac fermions.

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

Dirac fermions





$$\boldsymbol{\delta}_1 = \frac{a}{2}(1,\sqrt{3}) \quad \boldsymbol{\delta}_2 = \frac{a}{2}(1,-\sqrt{3}) \quad \delta_3 = -a(1,0)$$

$$\boldsymbol{a}_1 = \frac{a}{2}(3,\sqrt{3}), \quad \boldsymbol{a}_2 = \frac{a}{2}(3,-\sqrt{3}) \qquad \boldsymbol{b}_1 = \frac{2\pi}{3a}(1,\sqrt{3}), \quad \boldsymbol{b}_2 = \frac{2\pi}{3a}(1,-\sqrt{3})$$

Dirac fermions

$$H = -t \sum_{\sigma,\ \alpha\in A} \sum_{j=1}^{3} \left(\psi_\sigma^\dagger(\mathbf{r}_\alpha)\psi_\sigma(\mathbf{r}_\alpha + \delta_j) + \psi_\sigma^\dagger(\mathbf{r}_\alpha + \delta_j)\psi_\sigma(\mathbf{r}_\alpha) \right)$$

$$t{=}2.7\ \text{eV}$$

$$\psi_{A\sigma}(\mathbf{k}) = \frac{1}{V} \sum_{N_i} \psi_\sigma(\delta_1 + \sum_{i=1,2} N_i \mathbf{a}_i) e^{i\mathbf{k}(\sum_{i=1,2} N_i \mathbf{a}_i)} e^{-i\mathbf{k}\delta_1}$$

$$\psi_{B\sigma}(\mathbf{k}) = \frac{1}{V} \sum_{M_i} \psi_\sigma(\sum_{i=1,2} M_i \mathbf{a}_i) e^{i\mathbf{k}(\sum_{i=1,2} M_i \mathbf{a}_i)}$$

$$H = -t \sum_{j=1}^{3} \int \frac{d^2k}{\Omega} \left(e^{i(\delta_j)\mathbf{k}} \psi_{\sigma B}^\dagger(\mathbf{k}) \psi_{\sigma A}(\mathbf{k}) + (c.c.) \right)$$

$$H = \int \frac{d^2k}{\Omega} \psi_\sigma^\dagger(\mathbf{k}) \hat{V} \psi_\sigma(\mathbf{k}), \quad \hat{V} = -t \begin{pmatrix} 0 & \sum_{j=1}^{3} e^{i(\delta_j)\mathbf{k}} \\ \sum_{j=1}^{3} e^{-i(\delta_j)\mathbf{k}} & 0 \end{pmatrix}$$

Dirac fermions

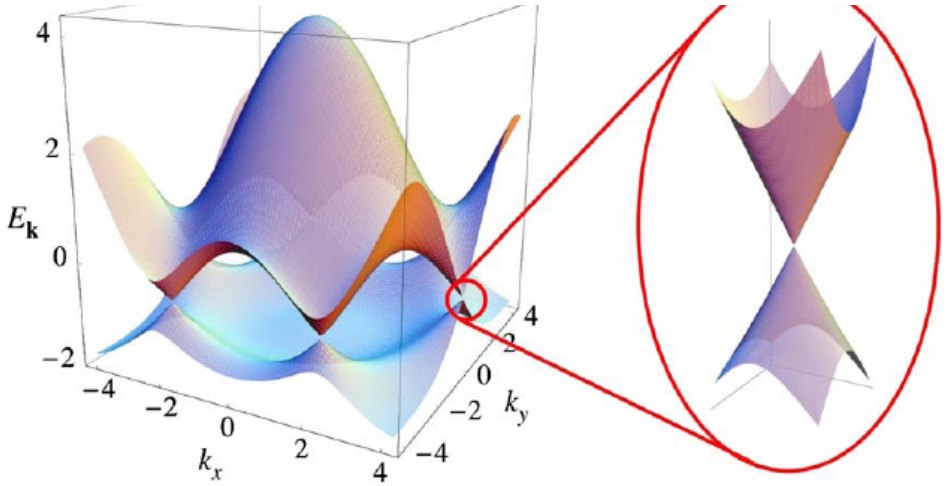
$$E_{\pm}(\mathbf{k}) = \pm t\sqrt{3 + f(\mathbf{k})} - t' f(\mathbf{k})$$

$$f(\mathbf{k}) = 2\cos(\sqrt{3}k_y a) + 4\cos\left(\frac{\sqrt{3}}{2}k_y a\right)\cos\left(\frac{3}{2}k_x a\right)$$

$$\boldsymbol{K} = \left(\frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a}\right), \quad \boldsymbol{K}' = \left(\frac{2\pi}{3a}, -\frac{2\pi}{3\sqrt{3}a}\right)$$

Near the K-points:

$$\hat{V}_{\pm}(\mathbf{q}) = \frac{3ta}{2}\begin{pmatrix} 0 & iq_1 \pm q_2 \\ -iq_1 \pm q_2 & 0 \end{pmatrix} = v_F(-\sigma_2 q_1 \pm \sigma_1 q_2)$$



Dirac fermions

$$\psi_\sigma \equiv \begin{pmatrix} \psi^+_{\sigma A} \\ \psi^+_{\sigma B} \\ \psi^-_{\sigma A} \\ \psi^-_{\sigma B} \end{pmatrix}$$

$$H = \int \frac{d^2q}{\Omega} \psi^\dagger_\sigma(\mathbf{q}) \hat{D} \psi_\sigma(\mathbf{q}) \qquad \hat{D} = \begin{pmatrix} \hat{V}_+(\mathbf{q}) & 0 \\ 0 & \hat{V}_-(\mathbf{q}) \end{pmatrix}$$

$$H = \int d^2x \psi^\dagger_\sigma(\mathbf{x}) \hat{D} \psi_\sigma(\mathbf{x})$$

$$\hat{D} = -iv_F \gamma^0 \gamma^a \partial_a, \; a = 1, 2$$

Low-energy effective field model

The action:

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

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

The Fine Structure Constant for graphene in vacuum: $\alpha = 300/127 \sim 2.$

Low energy effective field model is a quantum field theory with very strong interaction.

Another consequence of the small v_F/c ratio*:* we can neglect the retardation and take into account only electrical field. After it the action takes the form:

$$S_{Eucl.} = \frac{1}{2}\int \sum_{i=1,2,3}(\partial_4 A_i - \partial_i A_4)^2 d^3xd\tau + \sum_{a=1,2}\left(\int \overline{\psi}_a(\partial_4 + i\frac{e}{\sqrt{v_F}}A_4)\gamma_4\psi_a d^2xd\tau\right)$$

Coulomb interaction in graphene

The strength of the Coulomb interaction in graphene can be controlled by the surrounding media or a substrate under the graphene sheet. In case of a substrate with dielectric permittivity ε the value of the effective Fine Structure constant is

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

Therefore, it is possible to study the effective field theory experimentally both in strong-coupling and in small-coupling regime. The smaller the dielectric permittivity of the substrate, the larger is the effective coupling constant. The strongest interaction can be observed in the free graphene in vacuum.

Chiral symmetry breaking in graphene

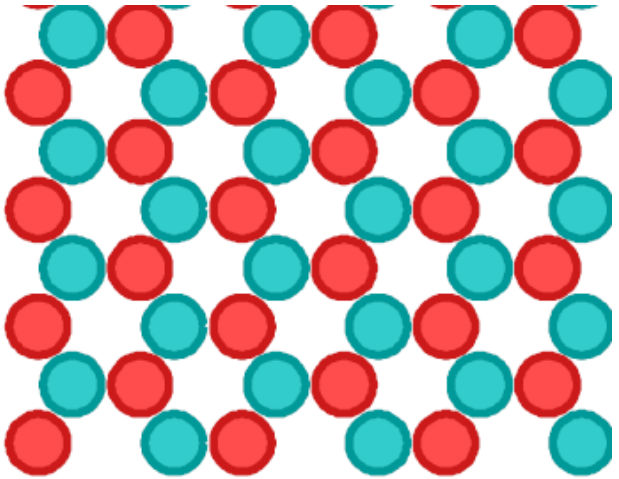
Symmetry group of the low-energy theory is U(4). Various channels of the symmetry breaking are possible. Two of them are studied at the moment. They correspond to 2 different nonzero condensates:

$\bar{\psi}_a \sigma_3^{ab} \psi_b$ - antifferromagnetic condensate

$\bar{\psi}_a \psi_a$ - excitonic condensate

From microscopic point of view, these situations correspond to different spatial ordering of the electrons in graphene.

Antiferromagnetic condensate corresponds to opposite spin of electrons on different sublattices
Excitonic condensate indicates opposite charges on sublattices



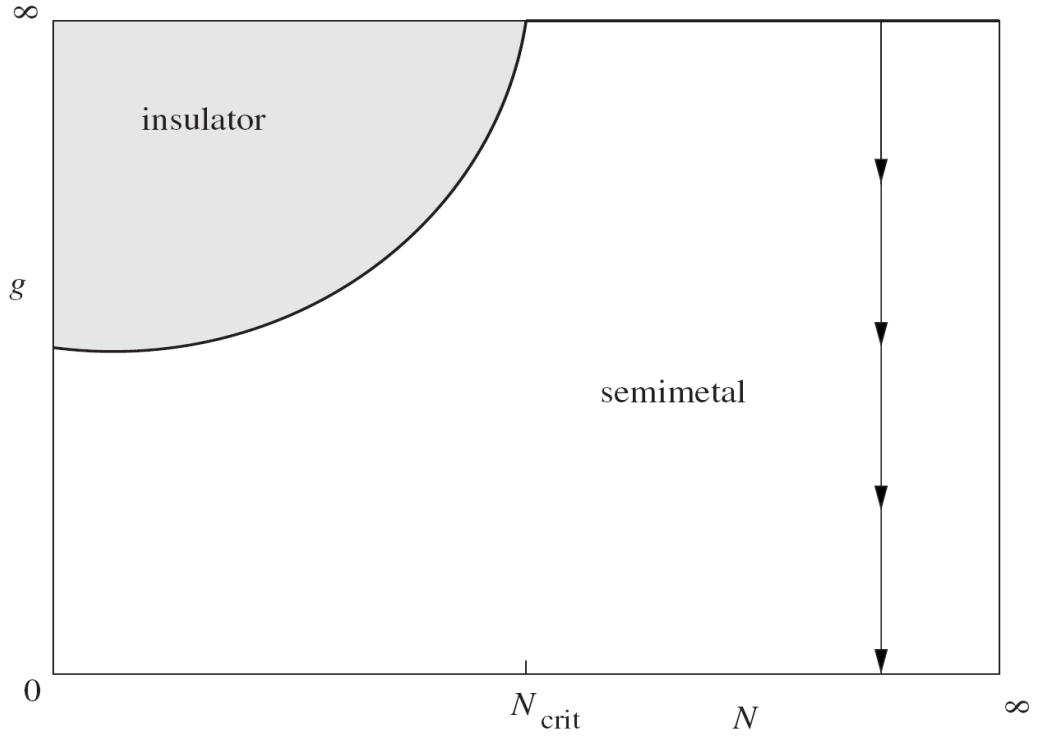
Chiral symmetry breaking in graphene: analytical study

1) E. V. Gorbar et. al., Phys. Rev. B 66 (2002), 045108.
$\alpha_c = 1{,}47$

2) O. V. Gamayun et. al., Phys. Rev. B 81 (2010), 075429.
$\alpha_c = 0{,}92$

3), 4)..... reported results in the region $\alpha_c = 0{,}7...3{,}0$

D. T. Son, Phys. Rev. B 75 (2007) 235423: large-N analysis:



Lattice formulation of the effective field model: gauge field

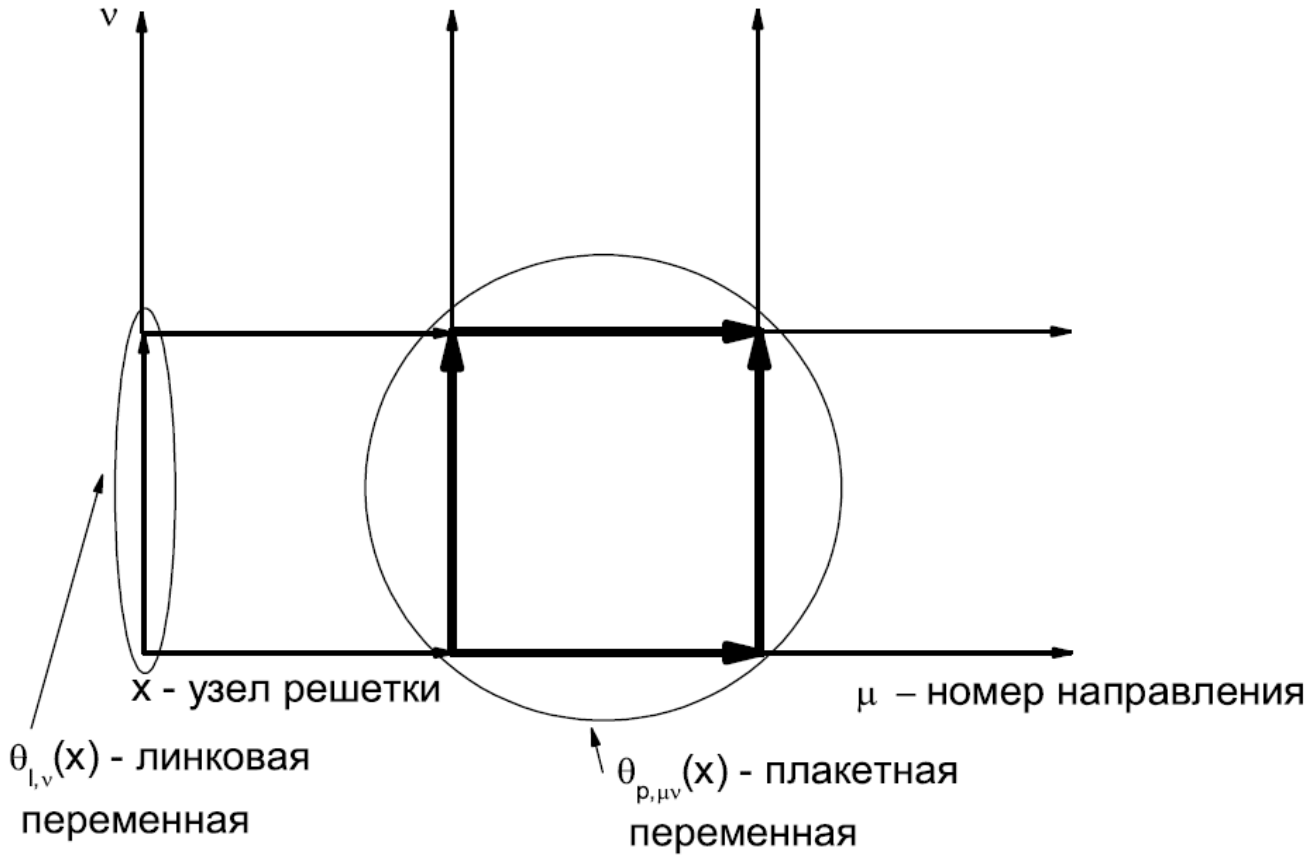
Noncompact lattice electrodynamics:

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

$$\theta_\mu(x) = \frac{e}{\sqrt{v_f}} a A_\mu$$

$$\Delta_\nu \theta_\mu(x) = \theta_\mu(x + \hat{\nu}) - \theta_\mu(x)$$

$$\theta_{\mu\nu}(x) = \Delta_\mu \theta_\nu(x) - \Delta_\nu \theta_\mu(x)$$



$$\beta = \frac{v_F}{e^2}$$

$$\beta = \frac{137}{300} \frac{1}{4\pi} \frac{\epsilon + 1}{2}$$

Lattice formulation of the effective field model: fermionic field

«Naive» lattice fermionic action (preserves chiral symmetry):

$$S_{naive} = \frac{1}{2a}\sum_{x,\hat{\mu}} (\bar{\psi}_x \gamma_\mu U_\mu(x) \psi_{x+\hat{\mu}} - \bar{\psi}_x \gamma_\mu U_\mu(x-\hat{\mu})^+ \psi_{x-\hat{\mu}}) + m\sum_x \bar{\psi}_x \psi_x$$

$$U_\mu(x) = e^{i\theta_\mu(x)}$$

The main problem: «Doublers» - this action describes in fact 16 fermionic fields in 3+1 space-time and 8 fermionic fields in 2+1 space-time

It is a well-known contradiction between preservation of the chiral symmetry and elimination of doublers (Nielsen-Ninomiya theorem)

Lattice formulation of the effective field model: fermionic field

Common solution in graphene simulations is so-called staggered fermions:

$$S = \frac{1}{2a}\sum_{x,\hat{\mu}} \bar{\chi}_x \alpha_\mu(x)\left(U_\mu(x)\chi_{x+\hat{\mu}} - U_\mu(x-\hat{\mu})^+ \chi_{x-\hat{\mu}}\right) + m\sum_x \bar{\chi}_x \chi_x$$

$$\alpha_\mu(x) = (-1)^{x_1+\ldots+x_{\mu-1}}$$

These action has only 2 doublers (which correspond to 2 flavours of the original continuous theory).

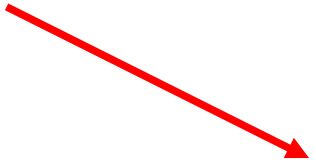
But: in the limit $m \to 0$ we have only U(1)*U(1) symmetry instead of the U(4).

Therefore, it's possible to study only excitonic condensate

$$\bar{\psi}_a \psi_a$$

Lattice calculations

Functional integrals



Lattice formulation

Monte-Carlo calculation of the multiple integrals

$$\int p(x) f(\vec{x}) d^n x = < f >$$

$$< f > = \frac{1}{N} \sum_{i=1}^{N} f(\vec{x}_i)$$

p(x) – probability distribution for the vector x.

Lattice calculations: fermionic determinant

Parition function:

$$\mathcal{Z} = \int \mathcal{D}\bar{\Psi}_x \, \mathcal{D}\Psi_x \, \mathcal{D}\theta_{x,0} \;\; \exp\left(-S_g\left[\theta_{x,0}\right] - S_\Psi\left[\bar{\Psi}_x, \Psi_x, \theta_{x,0}\right]\right) =$$

$$= \int \mathcal{D}\theta_{x,0} \, \det\left(D\left[\theta_{x,0}\right]\right) \exp\left(-S_g\left[\theta_{x,0}\right]\right).$$

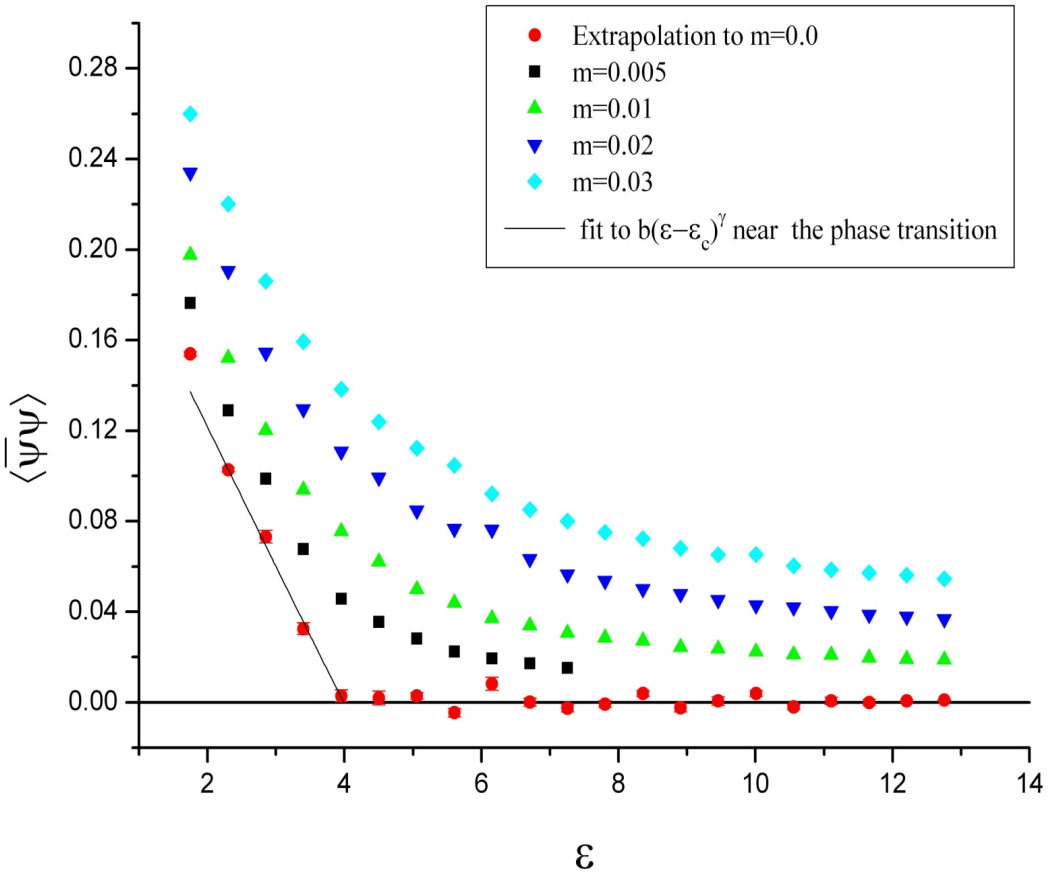
Fermionic determinant in case of staggered fermions:

$$D\left[\theta_{x,0}\right] = \begin{pmatrix} m & D_{eo} \\ D_{oe} & m \end{pmatrix} \qquad\qquad D_{eo}^\dagger = -D_{oe}$$

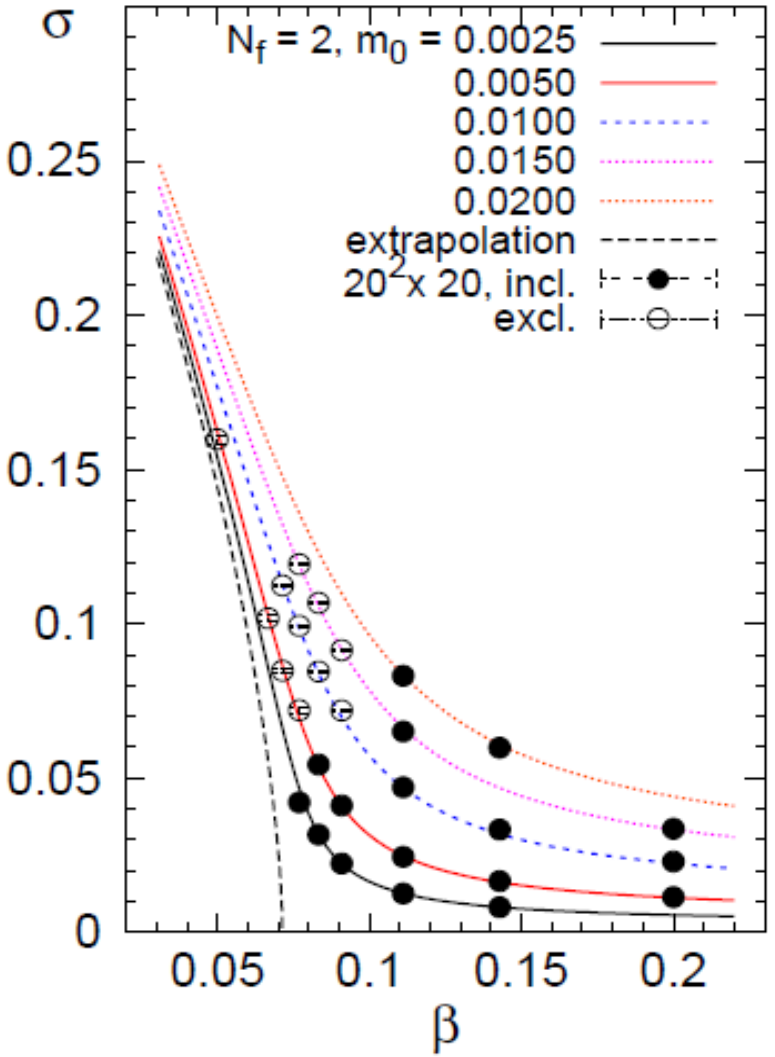
$$\det\left(D\right) = \det\left(m^2 + D_{eo}^\dagger \, D_{eo}\right)$$

$$\det\left(m^2 + D_{eo}^\dagger \, D_{eo}\right) = \int \mathcal{D}\bar{\phi}_x \, \mathcal{D}\phi_x \exp\left(-\sum_{x,y} \bar{\phi}_x \, \left(m^2 + D_{eo}^\dagger \, D_{eo}\right)_{x,y}^{-1} \phi_y\right)$$

Excitonic condensate



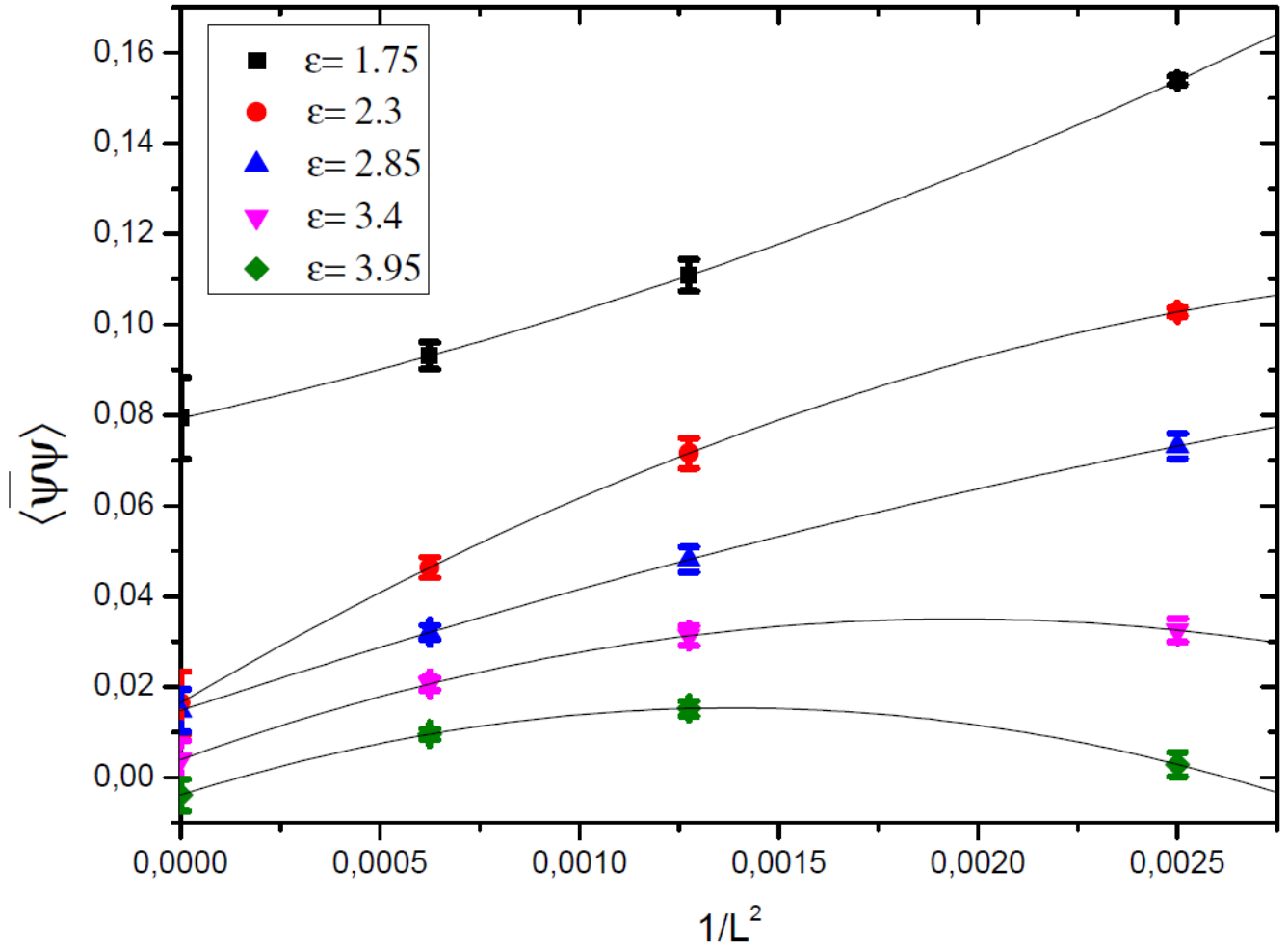
P. V. Buividovich et. al., Phys. Rev. B 86 (2012), 045107.



Joaquín E. Drut, Timo A. Lähde, Phys. Rev. B 79, 165425 (2009)

All calculations were performed on the lattice with 20^4 sites

Excitonic condensate: finite volume effects



In the infinite volume limit the phase transition is shifted to ε ~ 2.

Finite-volume effects need more careful study!

Calculation on the conductivity

Current-current correlator:

$$G_{ij}(\tau) = \int d^2x \langle J_i(0,0) J_j(x,\tau) \rangle$$

$$J_i = \bar{\psi} \Gamma_i \psi$$

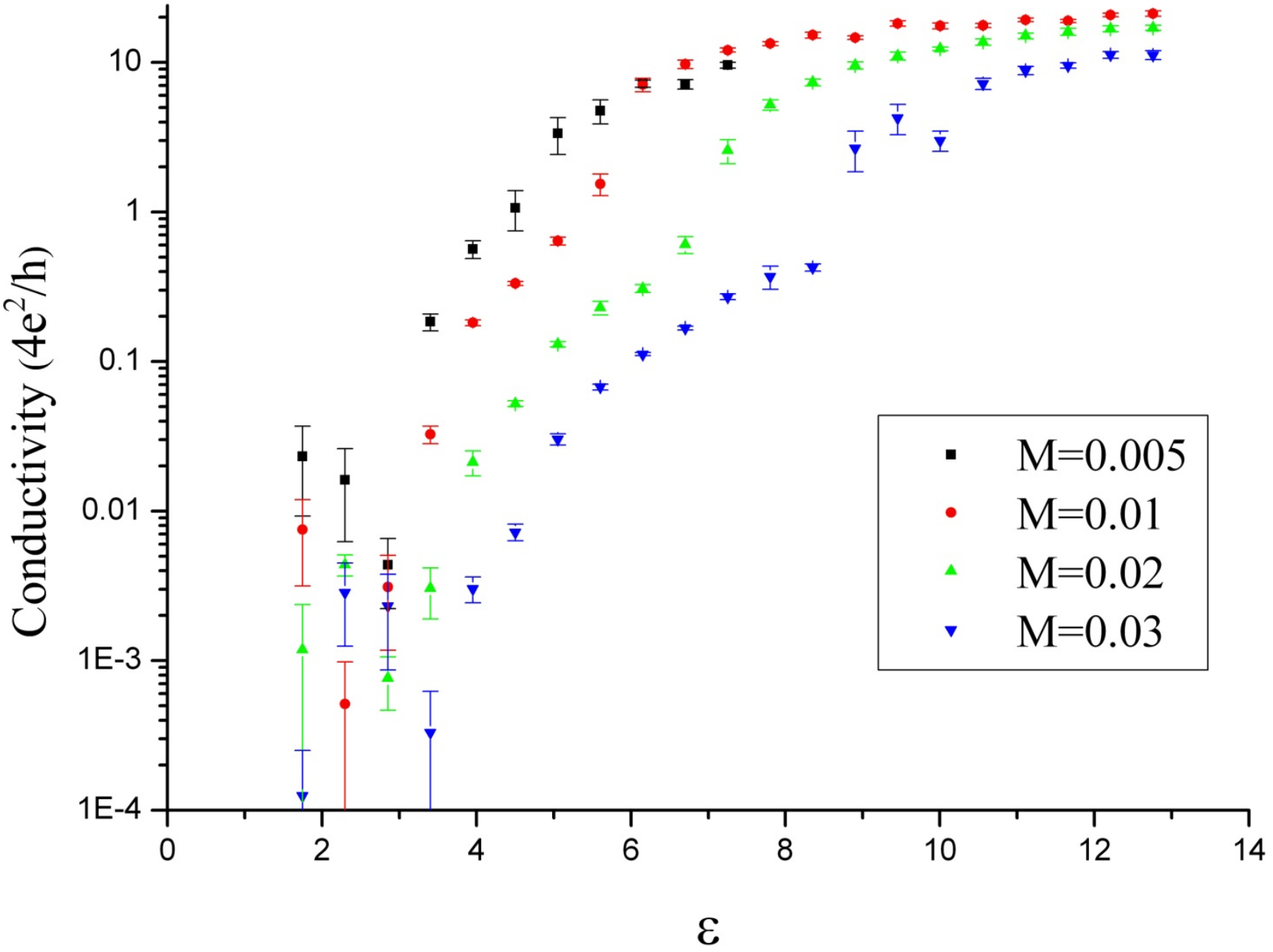
Spectral function:

$$G_{ij}(\tau) = \int_0^\infty dw K(w,\tau) \rho_{ij}(\tau)$$

$$K(w,\tau) = \frac{w}{2T} \frac{\cosh(w(\tau - 1/2T))}{\sinh(w/2T)}$$

Linear response theory: $\sigma = \dfrac{\rho_{ii}}{2T}$

Conductivity



P. V. Buividovich et. al., Phys. Rev. B 86 (2012), 045107.

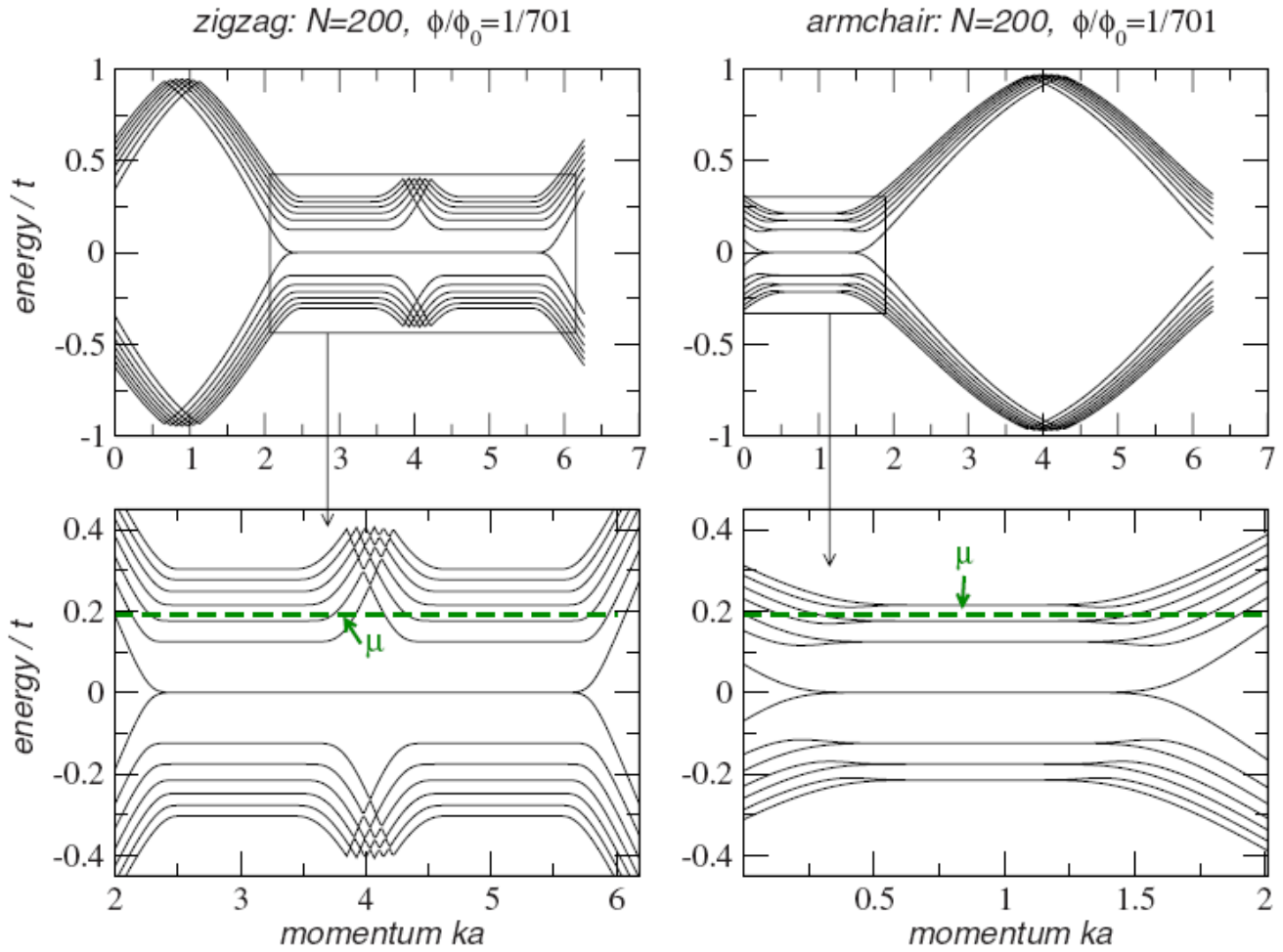
Conclusions

Electronic excitations in graphene in low-energy limit can be described as 2 flavours of massless Dirac fermions strongly interacting with each other by the Coulomb interaction. We can neglect retardation of the electromagnetic field

There are some predictions of the chiral phase transition in graphene with generation of the excitonic condensate. From microscopic point of view this condensate corresponds to the charge separation between sublattices. All theoretical predictions have been done within the effective low-energy theory.

Analtycal predictions give conflicting results. Lattice calculations need more careful study of the finite-volume effects. In the infinite-volume limit phase transirion seems to be around dielectric permittivity of a substrate ~2.

Graphene in magnetic field



A. H. Castro Neto, Rev. Mod. Phys. 81, 109–162 (2009)

External magnetic field causes increase of density of states near the fermi-point. It can potentially decrease the critical coupling constant.

Graphene in magnetic field: analytical predictions

1) E. V. Gorbar et. al., Phys. Rev. B 66 (2002), 045108.
2) V. P. Gusynin, Phys. Rev. B 74, 195429 (2006)

$$\Delta - bL(B) f(\Delta, \mu) = 0.$$

$$L = \sqrt{\hbar v_F^2 |eB|/c}.$$

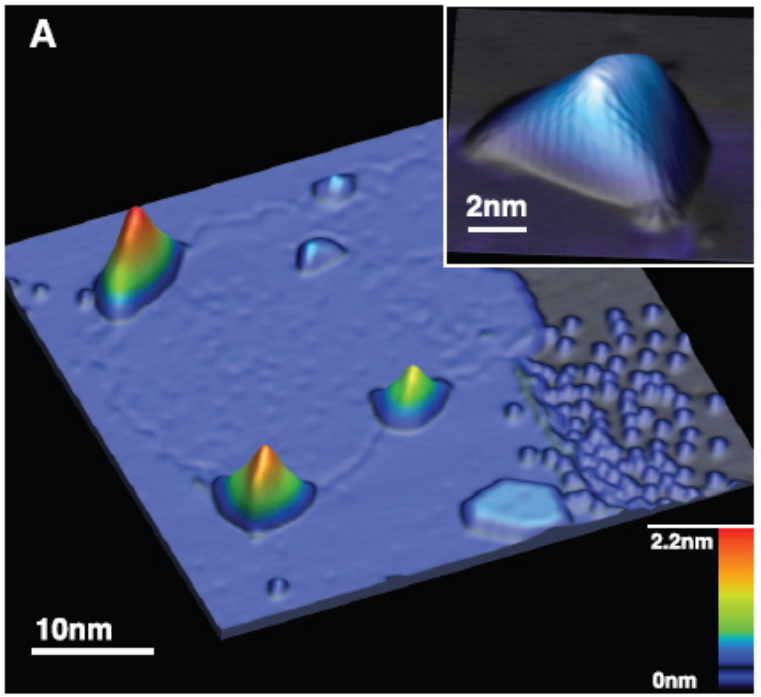
$$b = \frac{g}{\sqrt{2}} \int_0^\infty \frac{dk\, e^{-k^2}}{1 + k\chi_0}$$

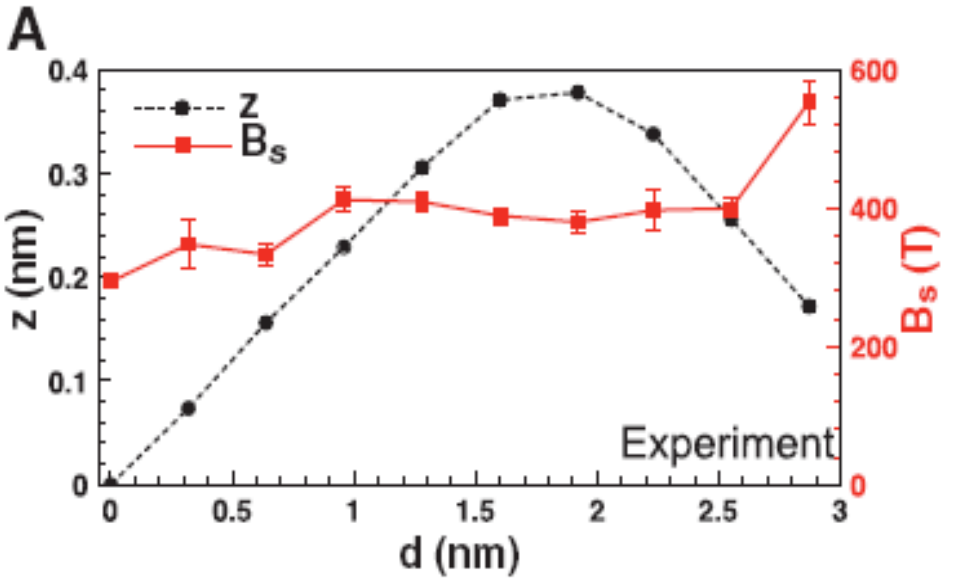
$$f(\Delta, \mu) = \frac{1}{\pi} \mathrm{Im} \left[\Psi \left(\frac{\gamma + i(\mu + \Delta)}{2\pi T} + \frac{1}{2} \right) - (\Delta \to -\Delta) \right]$$

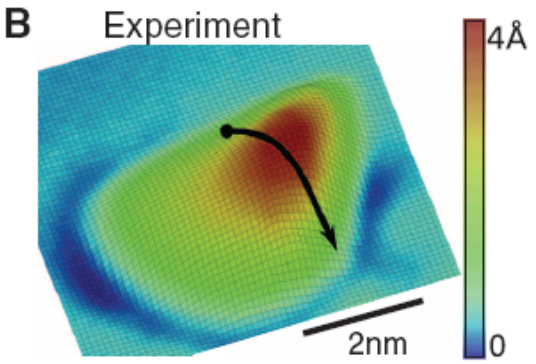
$$T = \mu = \gamma = 0 \qquad \Delta = bL(B)$$

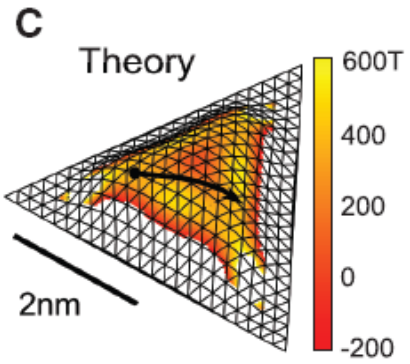
«Artificial» magnetic field

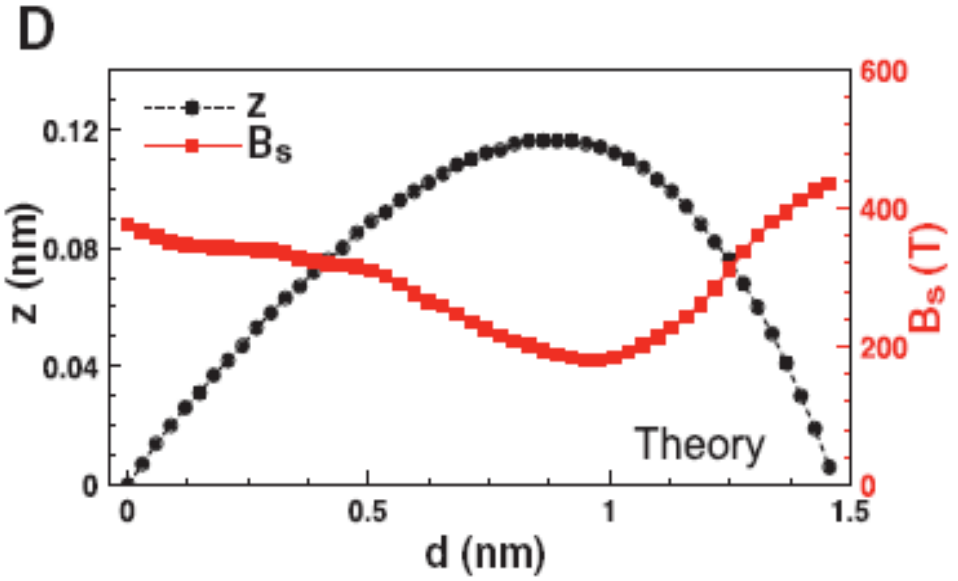
N. Levy et. al., Science 329 (2010), 544





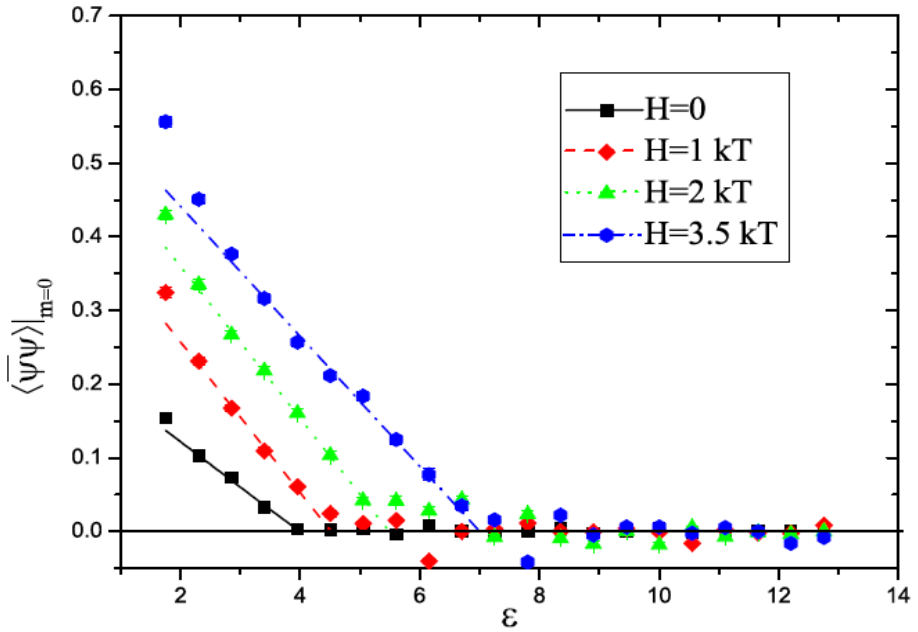


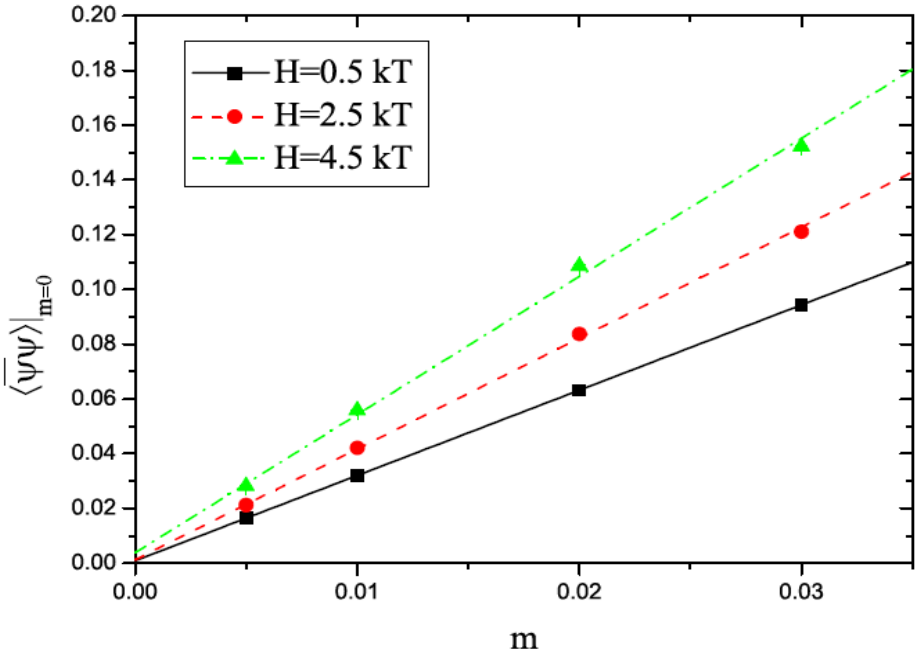




Graphene in magnetic field: lattice calculations

Excitonic condensate dependence on the coupling constant:

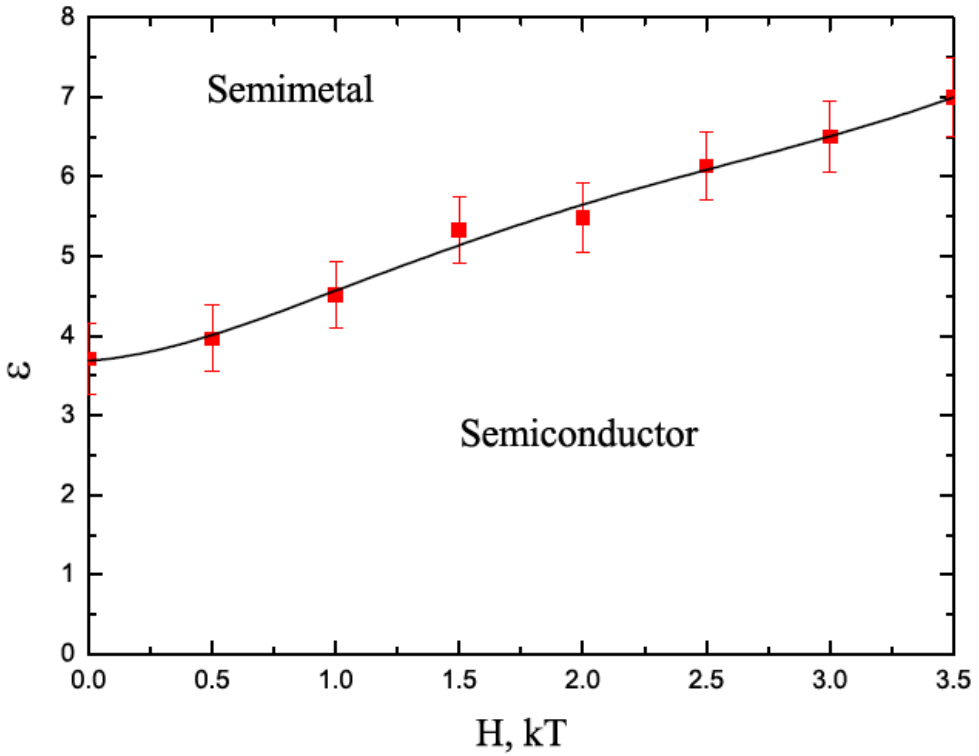




D. L. Boyda et. al., arXiv:1308.2814

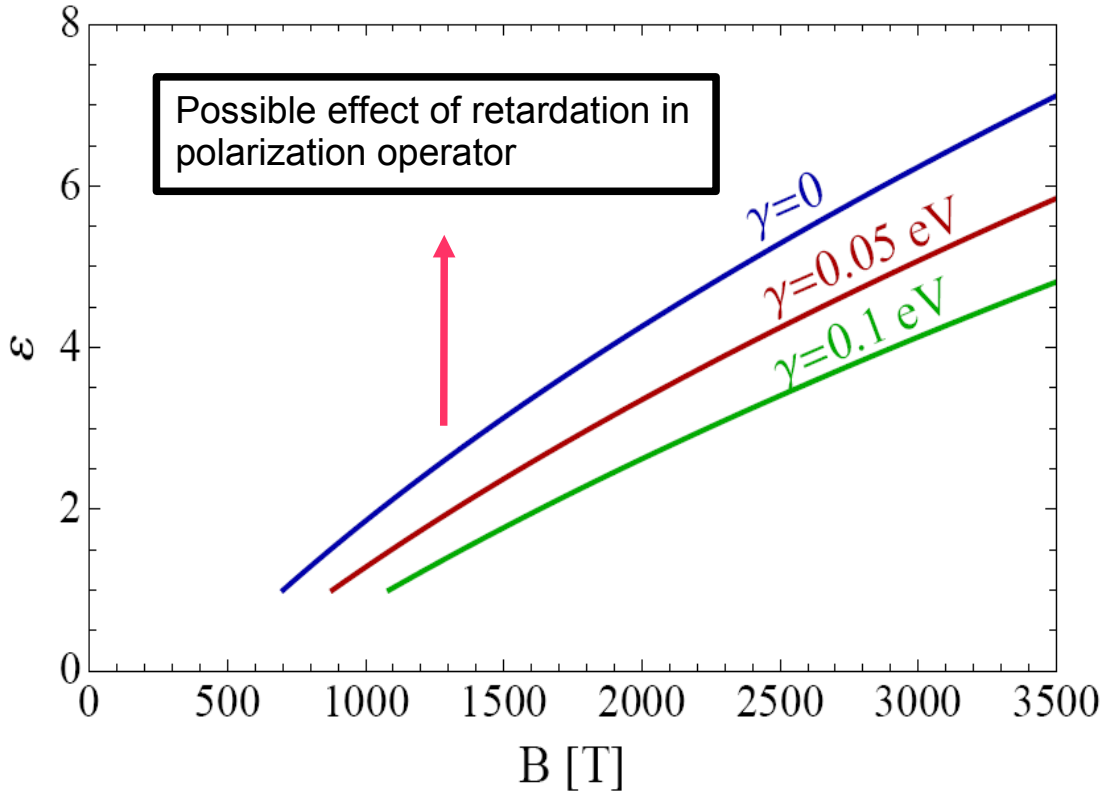
Phase diagram of graphene in external magnetic field: comparison of lattice simulations and analytical results

Lattice calculations:



D. L. Boyda et. al., arXiv:1308.2814

Analytical theory:



V. P. Gusynin, Phys. Rev. B 74, 195429 (2006)

Possible way to agreement between lattice and analytical calculations

Schwinger-Dyson equation for the fermionic propagator:

$$S^{-1}(p_0, \mathbf{p}) = p_0\gamma^0 - \mathbf{p}\boldsymbol{\gamma} - ie^2 \int \frac{d^3k}{(2\pi)^2} D(p_0 - k_0, \mathbf{p} - \mathbf{k})\gamma^0 S(k_0, \mathbf{k})\gamma^0$$

«Coulomb» propagator with loop corrections:

$$D(\omega, \mathbf{q}) = \frac{1}{|\mathbf{q}| + \Pi(\omega, \mathbf{q})}$$

One-loop approximation:

$$\Pi(\omega, \mathbf{k}) = \frac{\pi e^2 N_f}{4\kappa} \frac{\mathbf{k}^2}{\sqrt{\hbar^2 v_F^2 \mathbf{k}^2 - \omega^2}}$$

Subtraction of the ω dependence:

$$\Pi(\omega = 0, \mathbf{k}) = \frac{\pi e^2 N_f}{4\kappa\hbar v_F} |\mathbf{k}|$$

$$S^{-1}(p_0, \mathbf{p}) = Z^{-1} p_0\gamma^0 - A\mathbf{p}\boldsymbol{\gamma} - \Delta$$

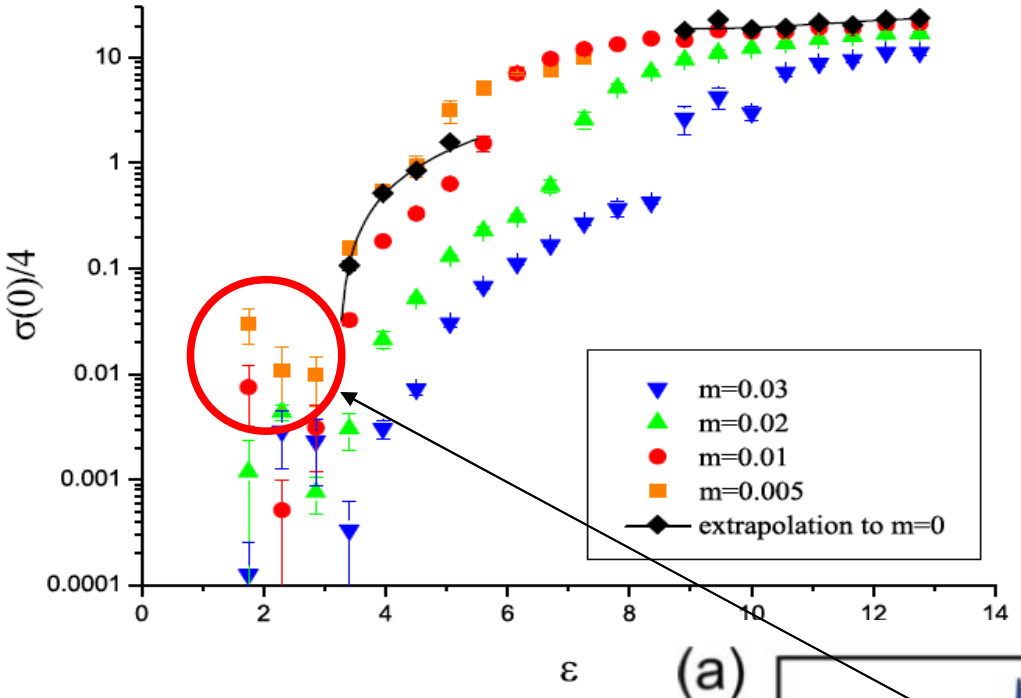
$$\Delta(p) = \Delta_0 + \frac{\alpha}{\pi^2} \int_0^\Lambda \frac{dk\, k\, \Delta(k)}{\sqrt{k^2 + \Delta^2(k)}} \mathcal{K}(p, k)$$

Conclusions

Magnetic field shifts the phase transition to the lower values of critical coupling constant. But the required magentic field is too strong for the experiment. Nevertheless, it is still possible to observe this shift in the curved graphene sheets where artificial magnetic field appears.
Agreement between analytical predictions and lattice calculations is still insufficient. Possible ways to bring them together are twofold:

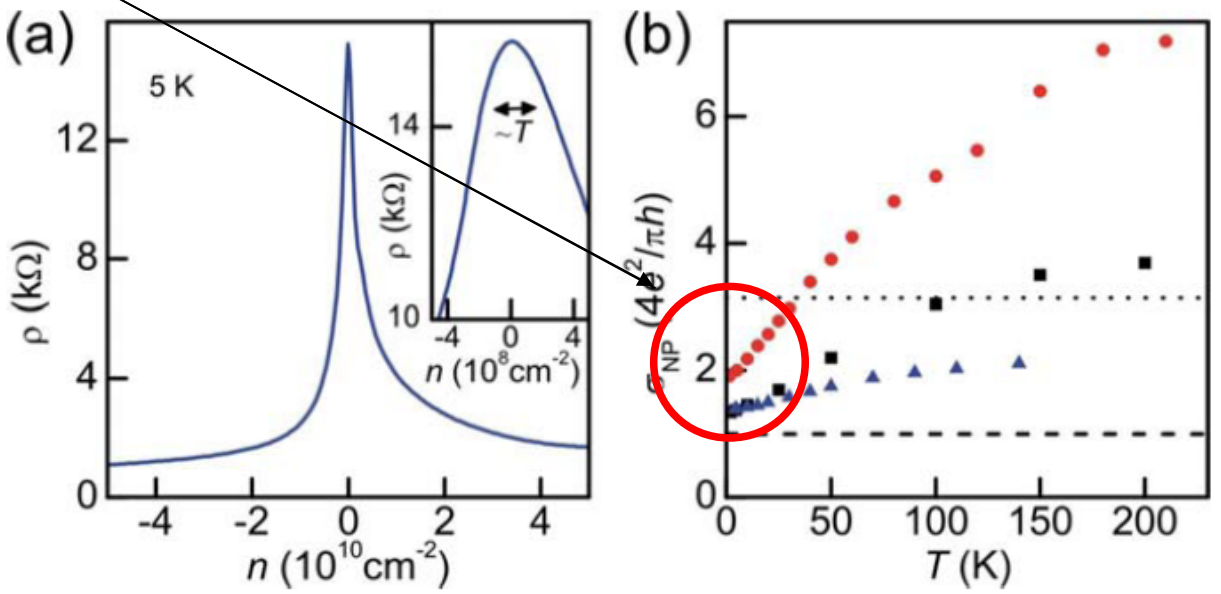
1) More accurate calculation of the polarization operator in the Schwinger-Dyson equation (namely, taking into account retardation effects in loop corrections).
2) Modification of lattice algorithms (better description of the chiral symmetry on the lattice, finite-size effects)

Graphene conductivity: theory and experiment



Lattice calculations: phase transition at ε=4

Experiment: D. C. Elias et. al., Nature Phys, 7, (2011), 701; No evidence of the phase transition



Tight-binding model on the honeycomb lattice

We start from the tight-binding hamiltonian on the original graphene honeycomb lattice:

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

where

$$\kappa = 2.7eV$$

$a^{+}_{x,s}$ - creation operator for the electron at the site x with the spin s

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

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:

Fermionic action and sign problem

Lattice fermionic action:

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

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

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

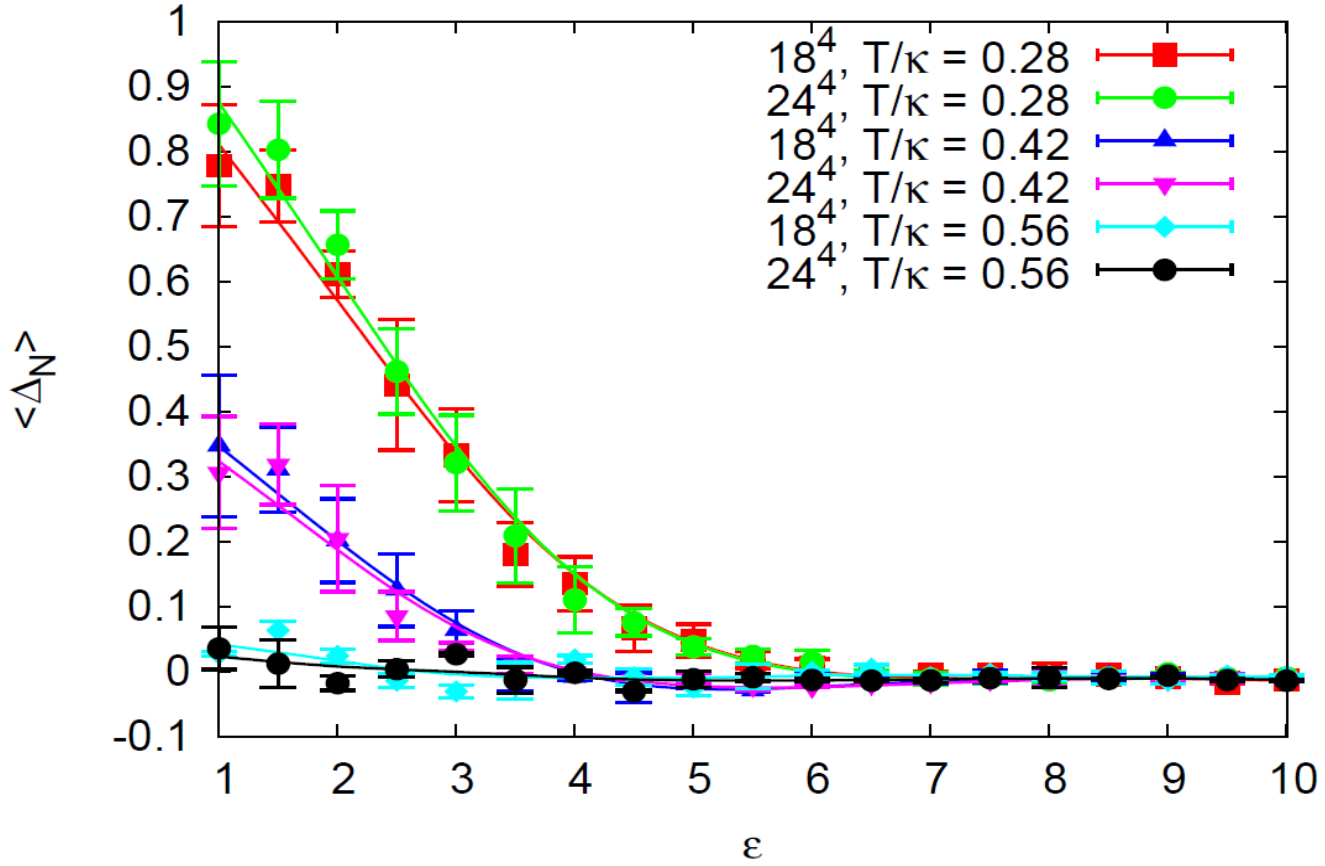
Partition function:

$$Tr(e^{-H\beta}) = \int \prod_{x,i} d\varphi^{(i)}_{x} e^{S_{Hubbard}} \det(MM^{+}) =$$

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

Antiferromagnetic phase transition

Due to the sign problem, it's impossible to simulate appearance of the excitonic condensate on the honeycomb lattice. Only antiferromagnetic condensate is studied at the moment.



Phase transition appears around ε ~ 2 in case of low temperatures. Free graphene is still in insulator phase.

P. V. Buividovich, M. I. Polikarpov, Phys. Rev. B 86 (2012) 245117

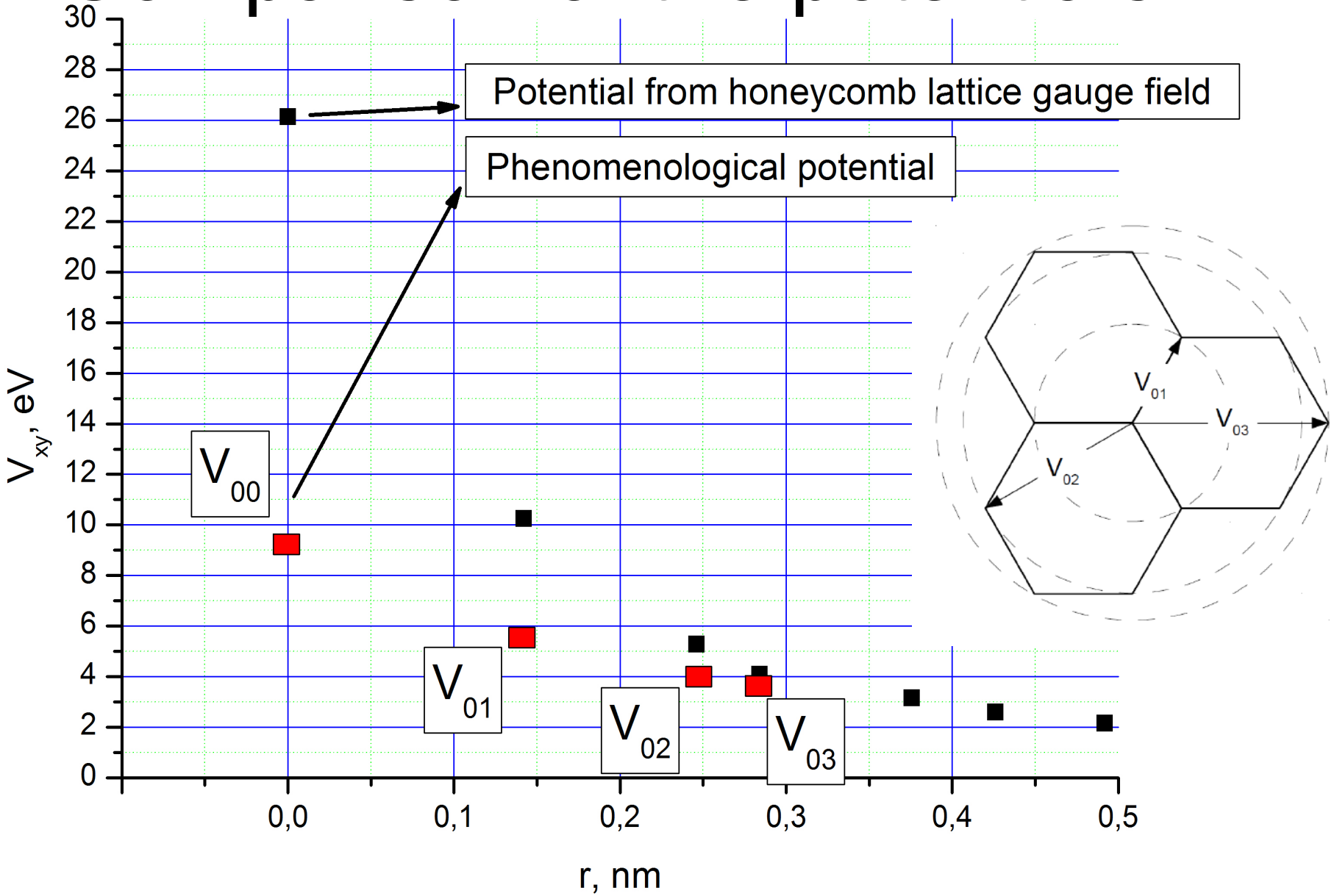
Coulomb interaction at small distances

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.

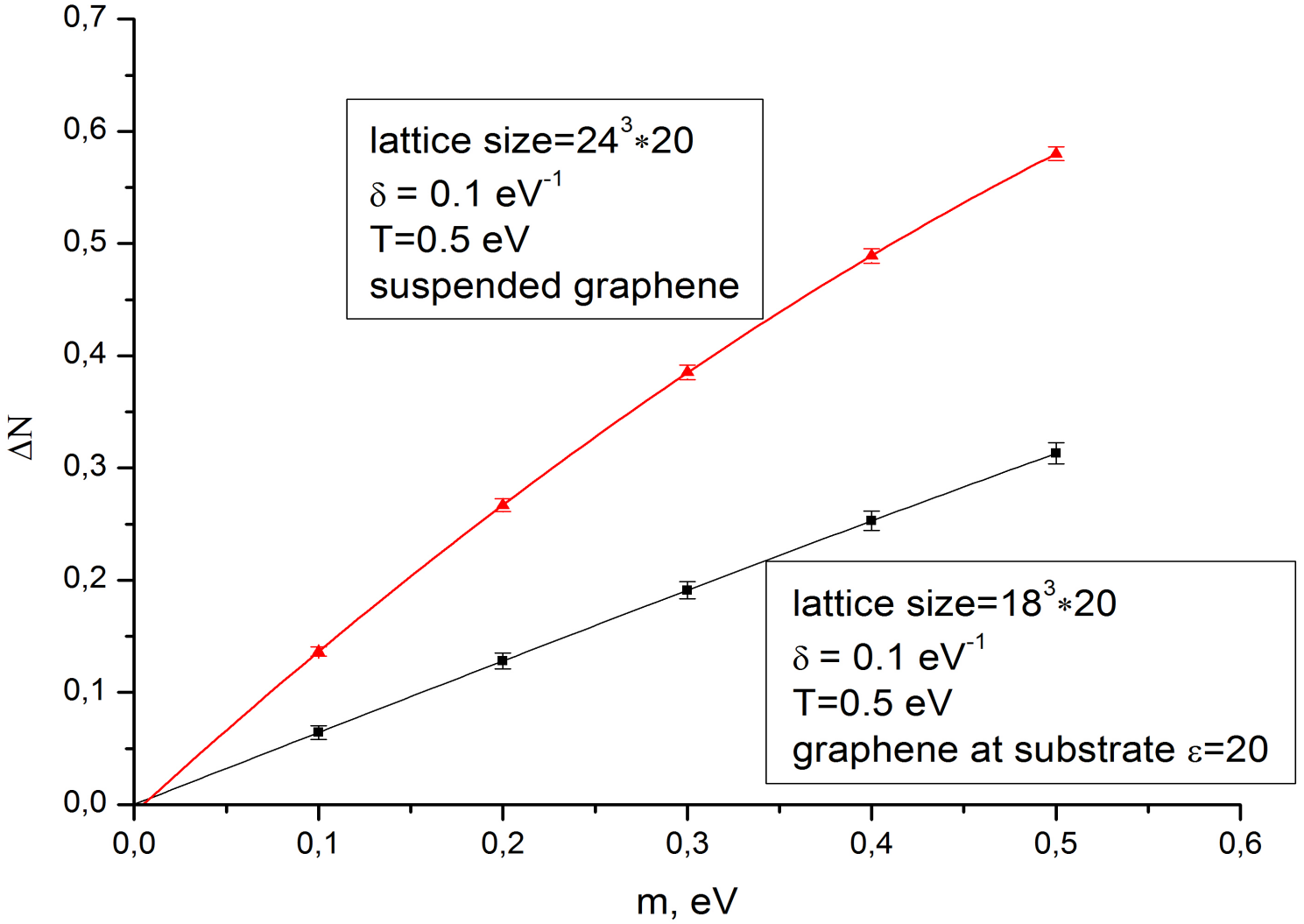
We tried to use the potentials calculated in the paper T. O. Wehling *et al.*, Phys. Rev. Lett. 106, 236805 (2011), where σ-orbitals were taken into account.

Comparison of the potentials



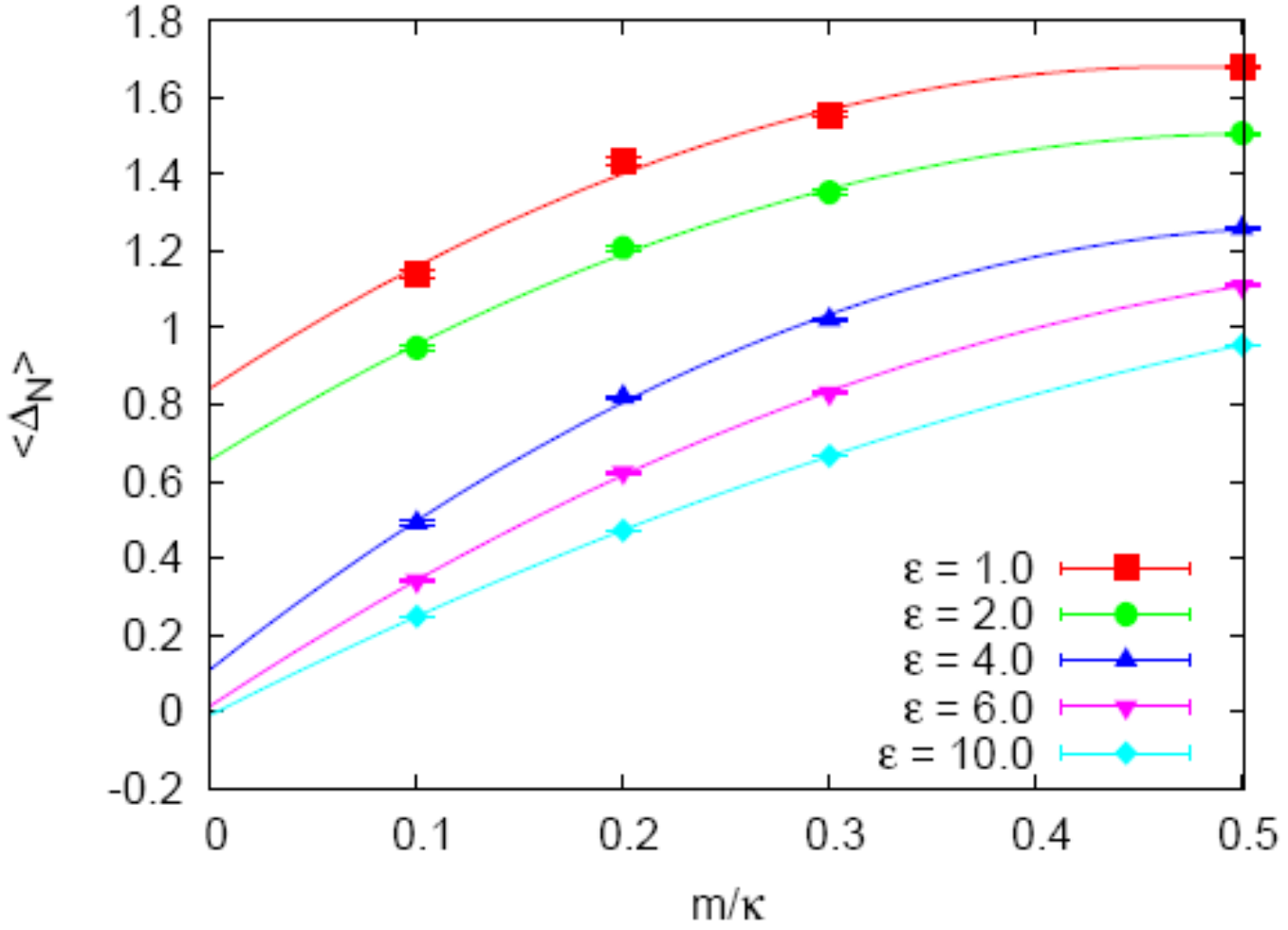
«Screening» of Coulomb interaction at small distances

Supression of the condensate. Free graphene is still a conductor



M. V. Ulybyshev et. al., Phys. Rev. Lett. 111, 056801 (2013)

Comparison with the calculations on the honeycomb lattice with non-screened Coulomb interaction

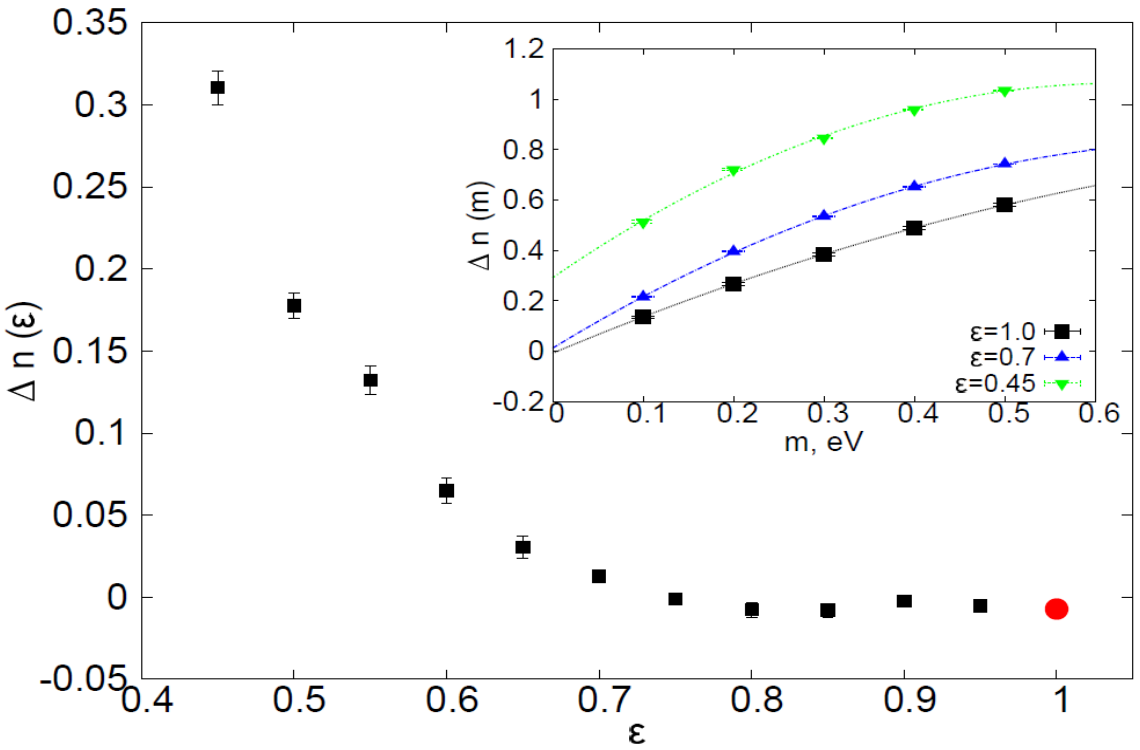


$T/\kappa = 0.28 \quad (\kappa\,\Delta\tau = 0.15)$

P. V. Buividovich, M. I. Polikarpov, Phys. Rev. B 86 (2012) 245117

Phase transition appears only in the region of unphysical values of coupling constant (ε<1)

M. V. Ulybyshev et. al., Phys. Rev. Lett. 111, 056801 (2013)



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

Very important point: recent calculations showed that antiferromagnetic phase transition is insensitive to the long-range interaction. It is caused only by short-range interactions.

Preliminary study of the excitonic phase transition on the honeycomb lattice

O. V. Pavlovsky et. al. arXiv:1311.2420, talk presented at Lattice 2013

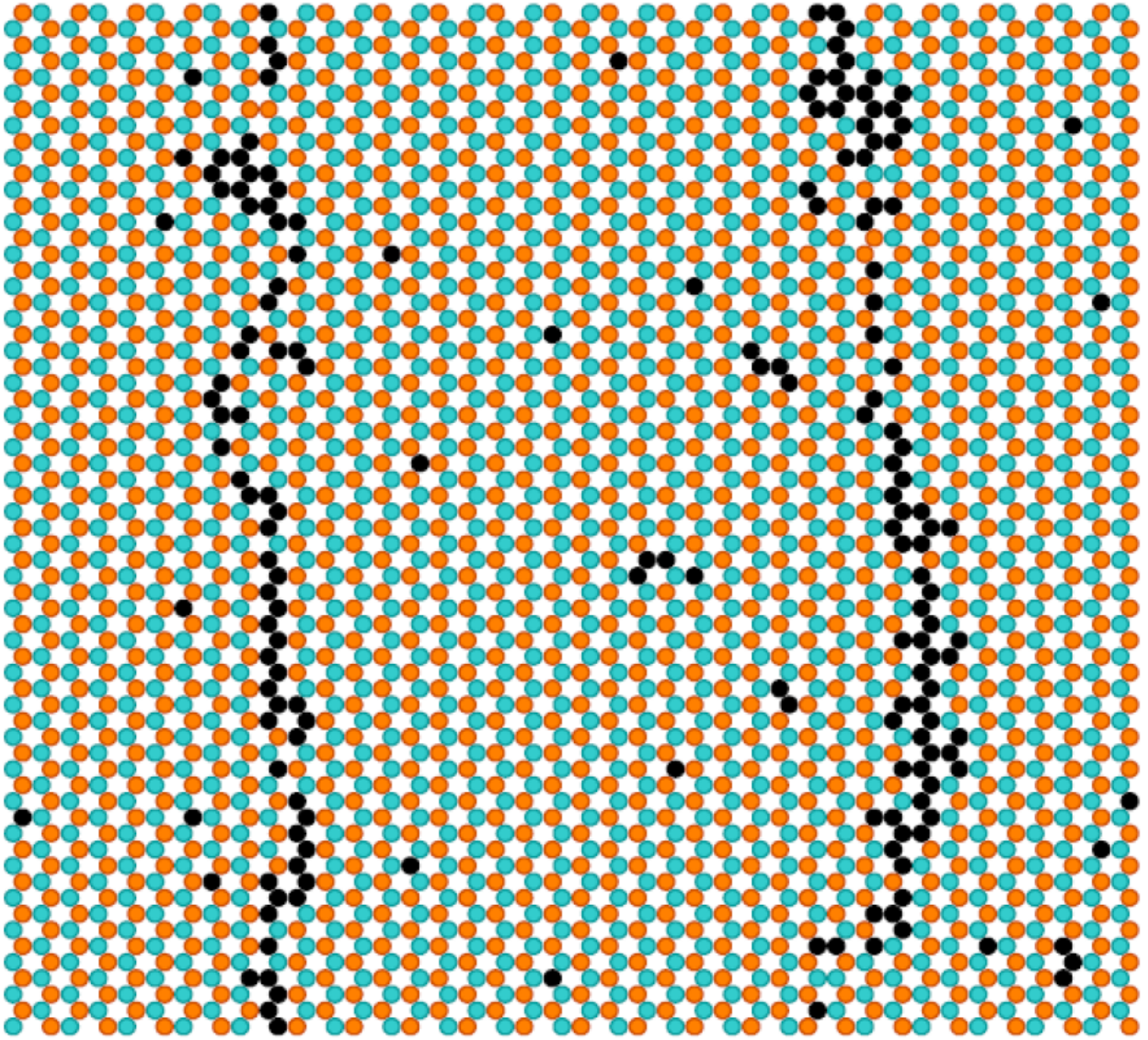
We can subtract hopping part of the hamiltonian and simulate simple statistical model:

$$H(\{q_x\}) = \sum_x V_{xx}(q_x)^2 + \sum_{x \neq y} V_{xy}(q_x)(q_y)$$

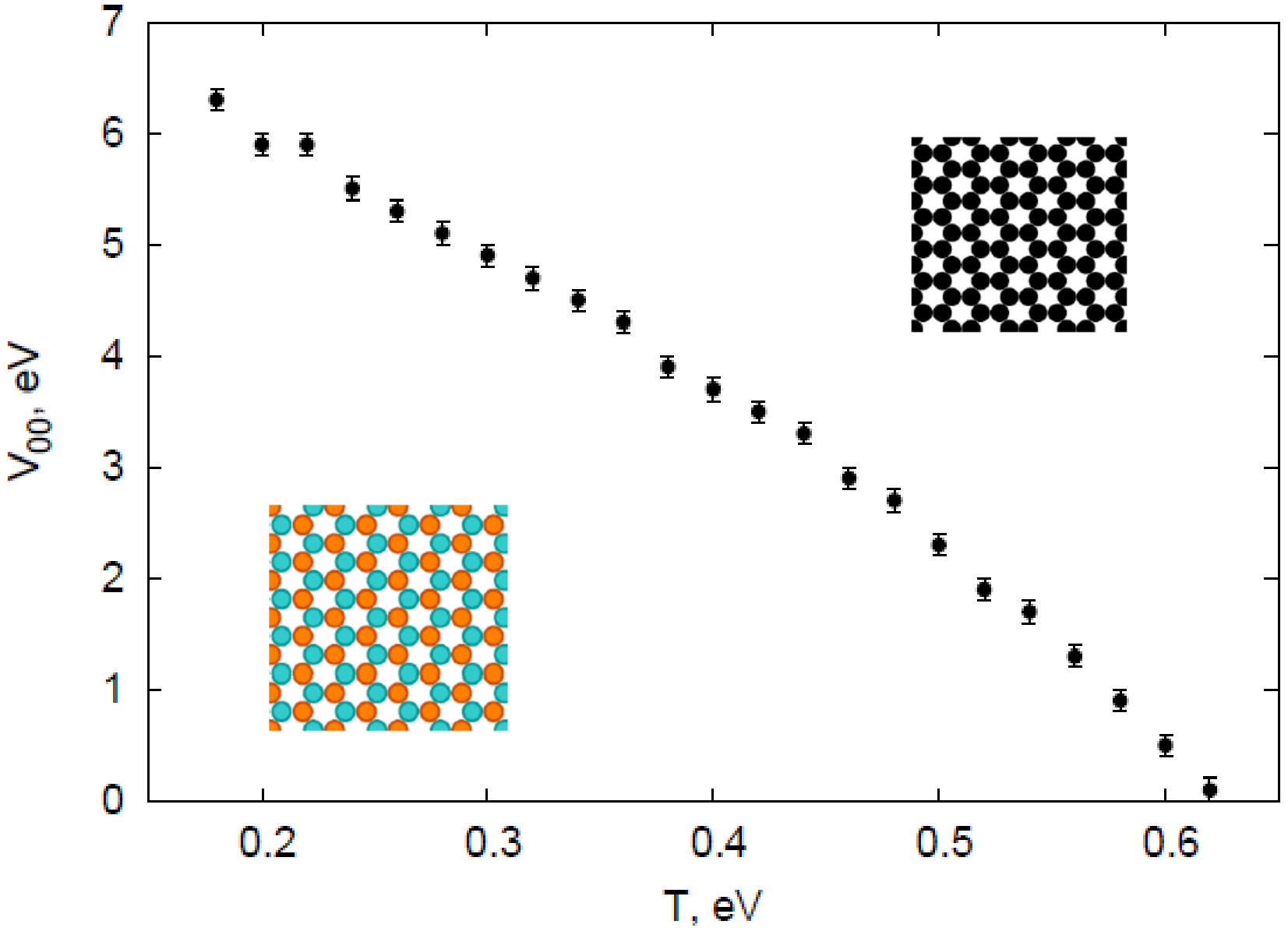
$$\langle O \rangle = \frac{\sum_{\{q_x\}} O(\{q_x\}) e^{-\beta H(\{q_x\})} \prod_x (1 + \delta_{q_x,0})}{\sum_{\{q_x\}} e^{-\beta H(\{q_x\})}}$$

We avoid sign problem because of the absence of the fermionic determinant in the action. In this simple model we can simulate spatial ordering of charge in graphene.

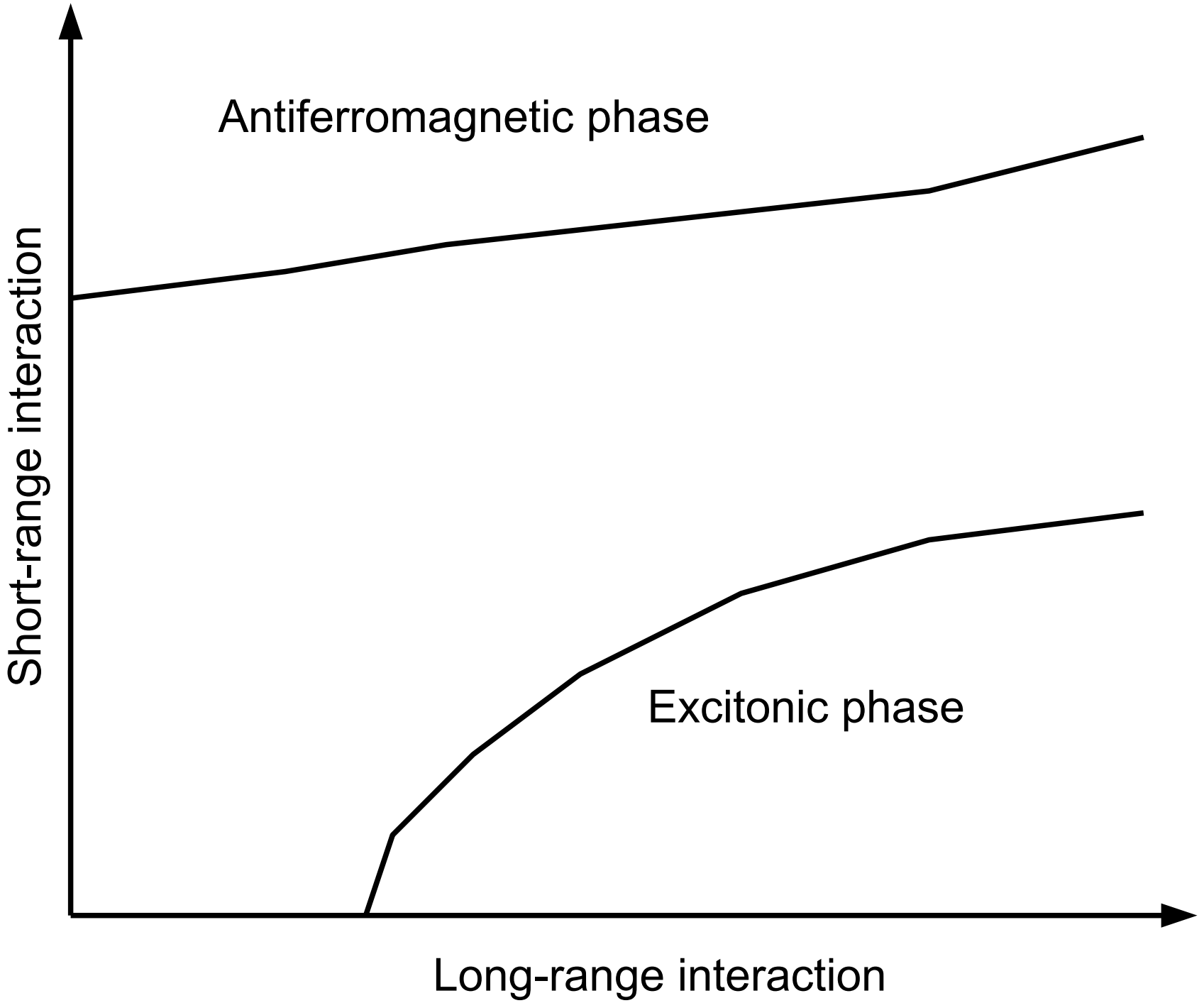
An example of the configuration of charges in the phase with broken sublattice (chiral) symmetry and nonzero excitonic condensate.



Phase diagram



We vary on-site interaction and temperature. All other potentials are constant and correspond to free graphene in vacuum


Antiferromagnetic phase
Excitonic phase
Short-range interaction
Long-range interaction

Summary: phase transitions in graphene, current situation from lattice simulations

1) We are able to simulate excitonic phase transition in low-energy effective theory and antiferromagnetic phase transition on the original honeycomb lattice.
2) Early simulations showed that both phase transitions appear around $\varepsilon \sim 4$. Now we understand that it's wrong! Antiferromagnetic phase transition is sensitive only to short-range interactions. Excitonic phase transition is sensitive both to short-range and long-range interactions.
3) Antiferromagnetic phase transition appears only when short-range interactions are ~1.5 times larger than in free graphene in vacuum.
4) Excitonic phase transition is still an open question. Simulations in effective field theory still show its existence at $\varepsilon \sim 2$. On-site interaction possibly suppress it to the unphysical region $\varepsilon < 1$, but this fact needs more careful study using simulations on the honeycomb lattice