Hybrid Monte Carlo simulations of Graphene in presence of vacancies

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Various channels of chiral symmetry breaking in graphene

Low energy effective theory: 2 flavors of 2+1D Dirac fermions and ordinary 3+1D U(1) gauge field.

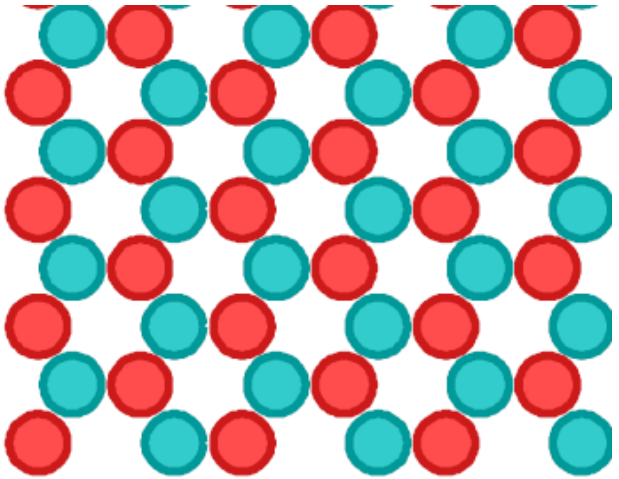
Symmetry group of the low-energy theory is U(4). Various channels of the symmetry breaking are possible. Two of them are studied at the moment. They correspond to 2 different nonzero condensates:

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

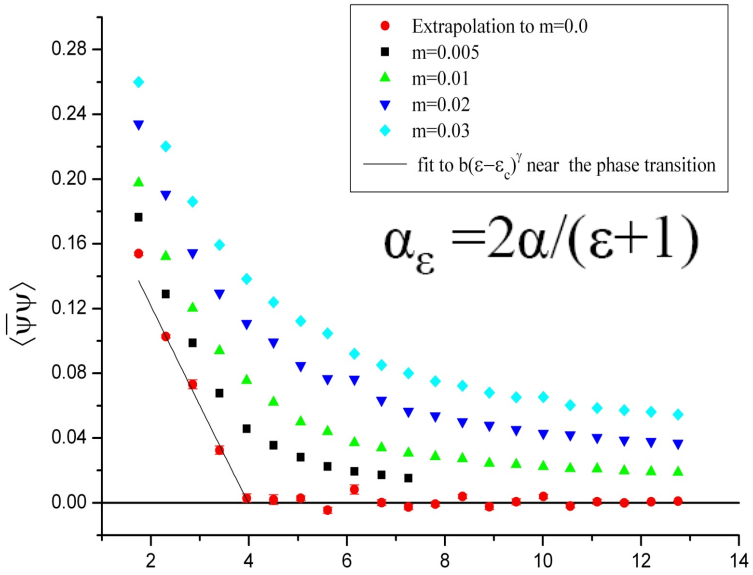
Antiferromagnetic condensate corresponds to opposite spin of electrons on different sublattices
Excitonic condensate indicates opposite charges on sublattices



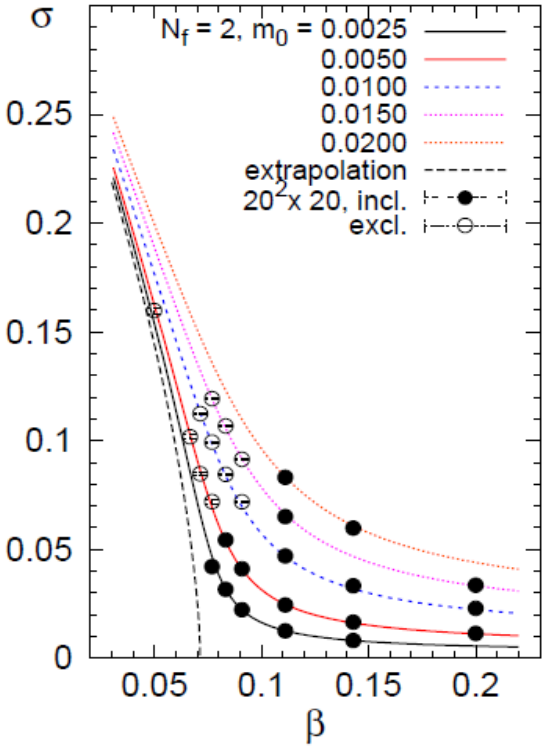
Excitonic phase transition

Studied analytically and on square lattice within the low-energy effective theory.

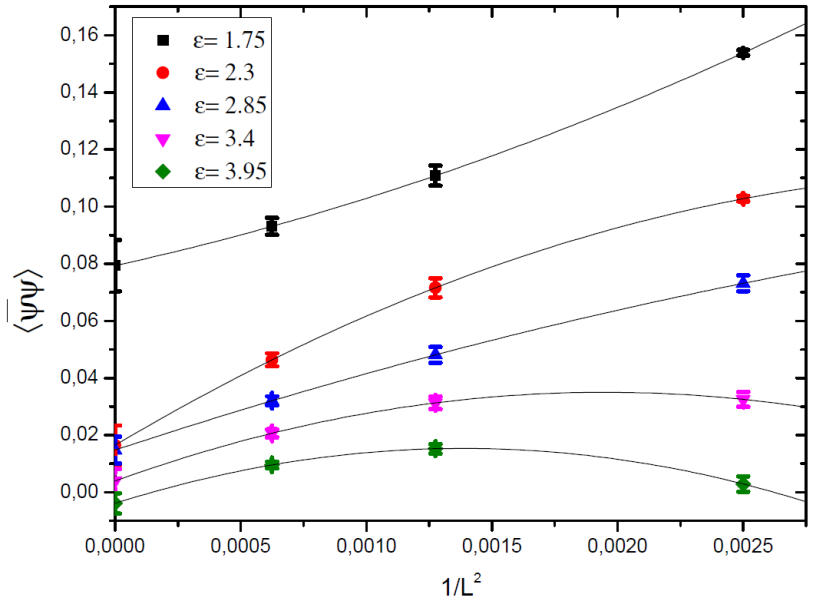
Lattice with 20^4 sites:



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



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



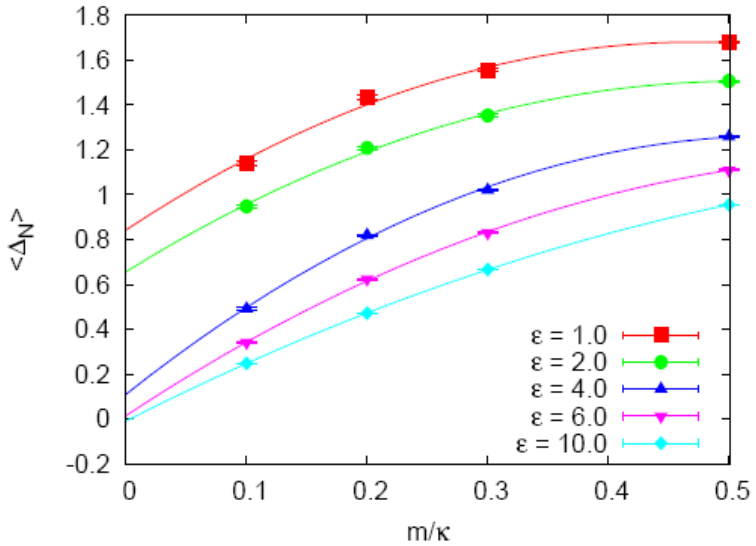
Probably large finite-volume effects!

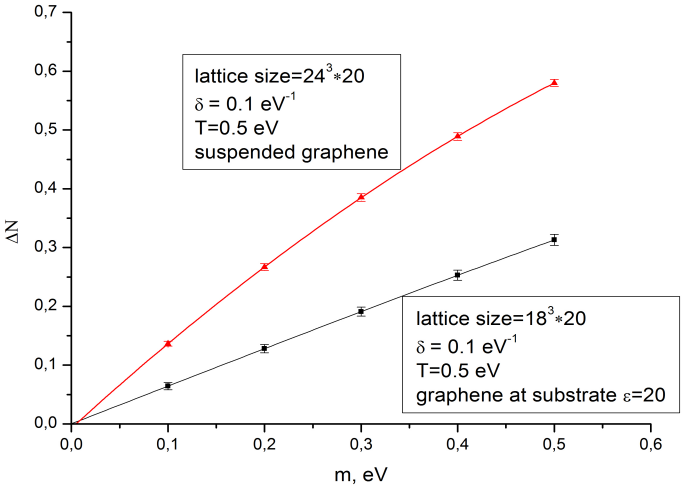
But the phase transition is still in the region ε>1. In means that suspended graphene is Predicted to be in the insulator phase

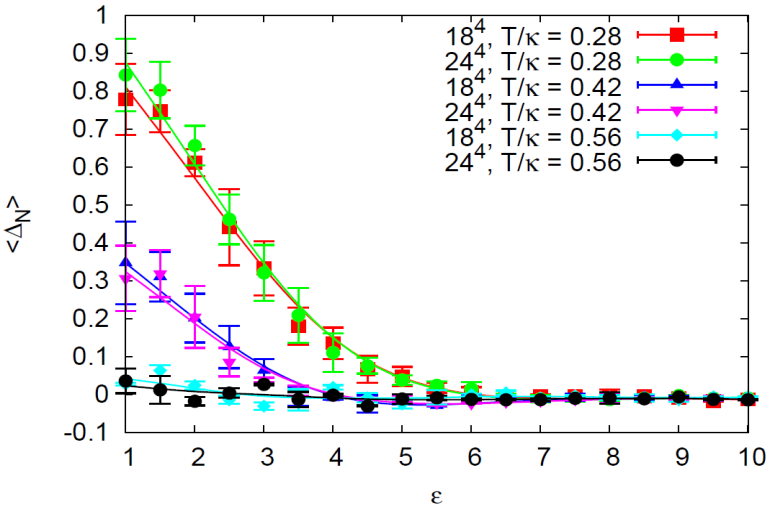
Antiferromagnetic phase transition

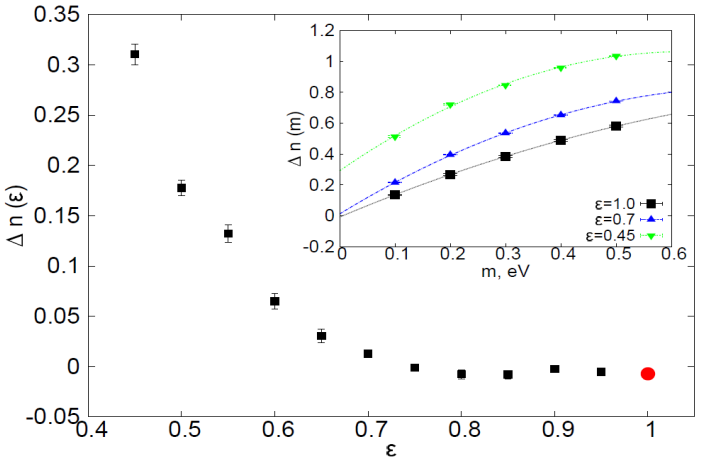
Studied numerically on original honeycomb lattice

$$\langle \Delta n \rangle = \frac{1}{N} \langle \sum (\hat{a}_x^\dagger \hat{a}_x + \hat{b}_x^\dagger \hat{b}_x) - \sum (\hat{a}_x^\dagger \hat{a}_x + \hat{b}_x^\dagger \hat{b}_x) \rangle$$







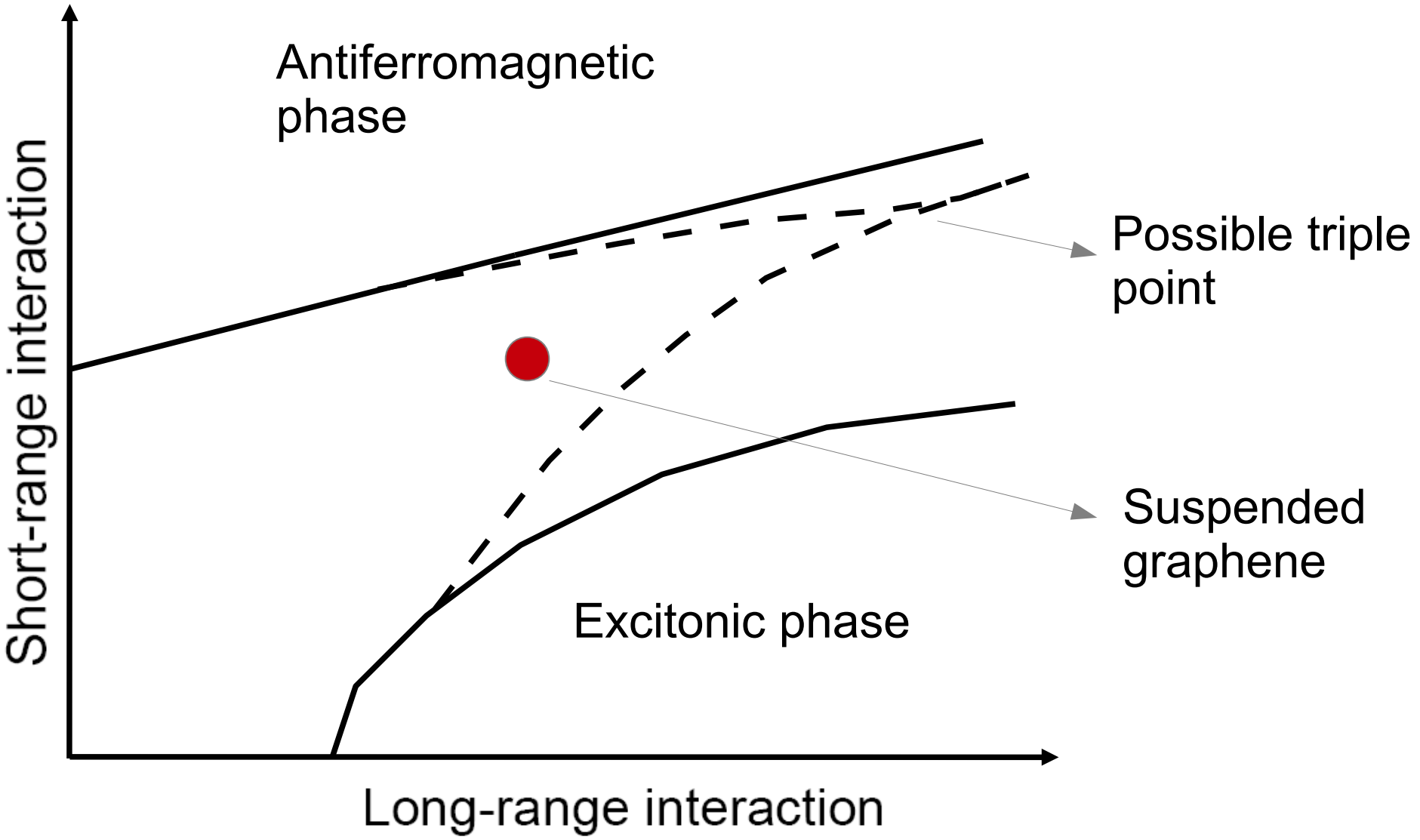


Lattice Coulomb interaction (P. V. Buividovich, M. I. Polikarpov, Phys. Rev. B 86 (2012) 245117)

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

Graphene phase diagram

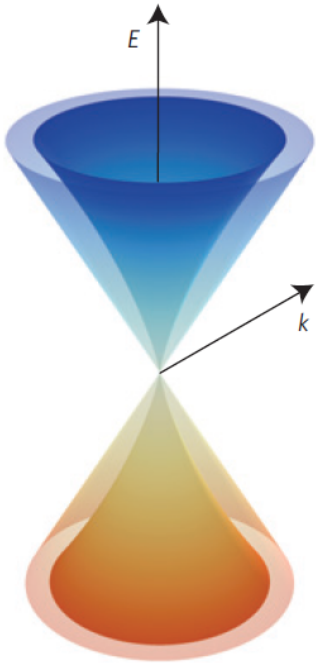
Influence of the short-range interactions on the excitonic phase transition:
O.V. Gamayun et. al. Phys. Rev. B 81, 075429 (2010).
Short-range repulsion suppresses formation of the excitonic condensate.

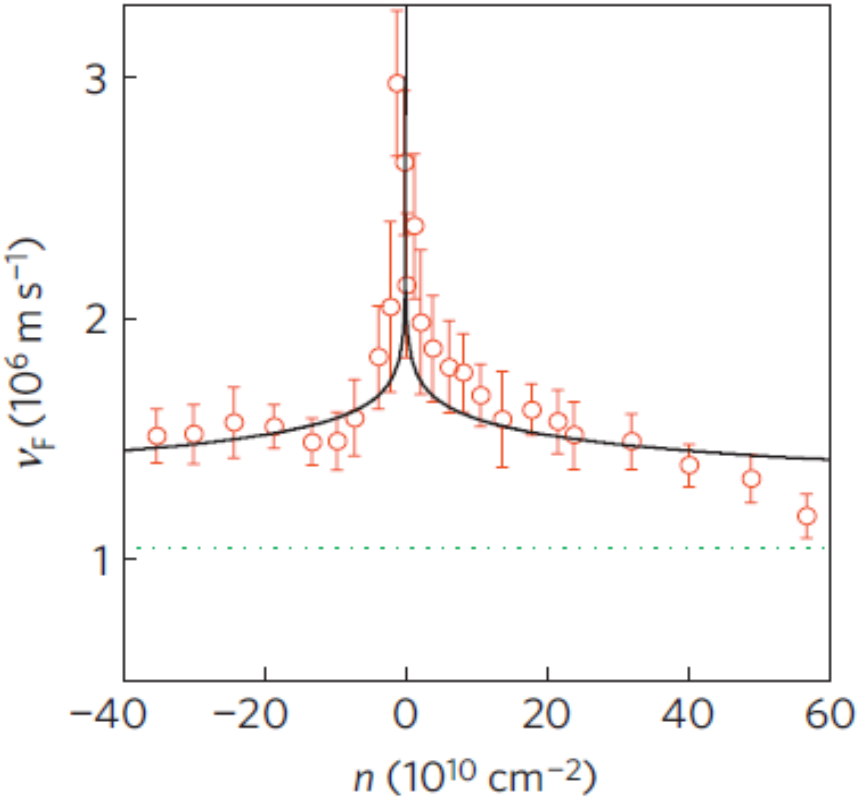


Can lattice field theory methods add something to the results of Density Functional Theory (DFT) calculations?

One of the interaction effects: Fermi velocity renormalization

Dirac cone in the vicinity of the K-point of Brillouine zone in presence of interaction:



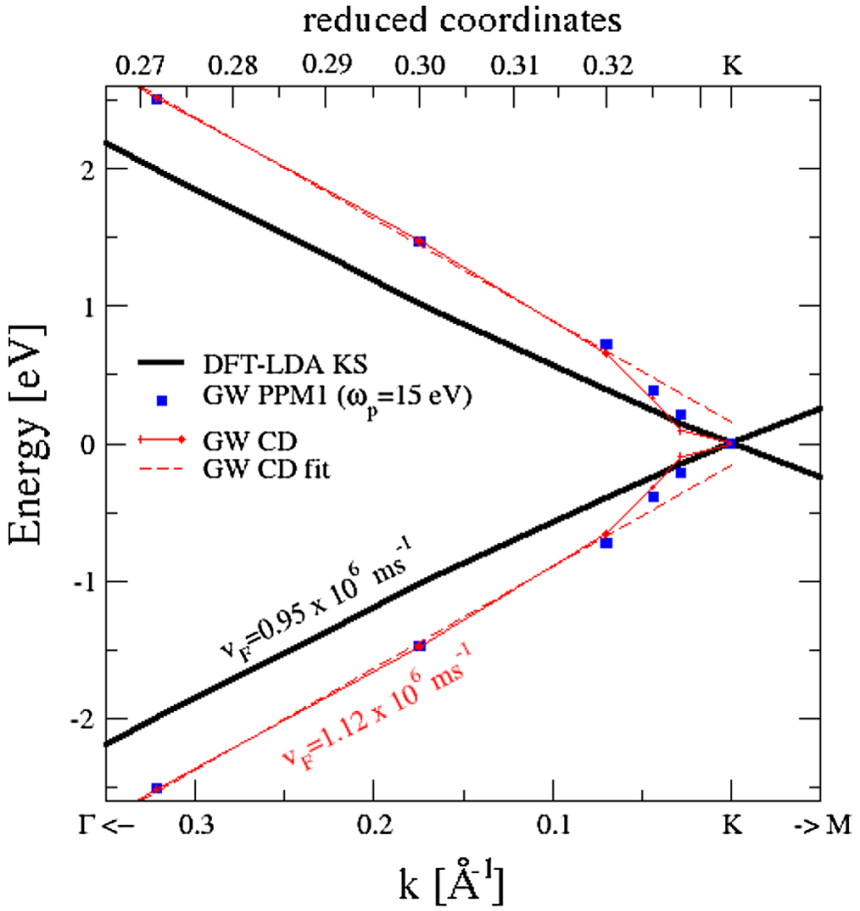


D. C. Elias et. al. Nature Physics 7 (2011), 701

Comparison with DFT calculations

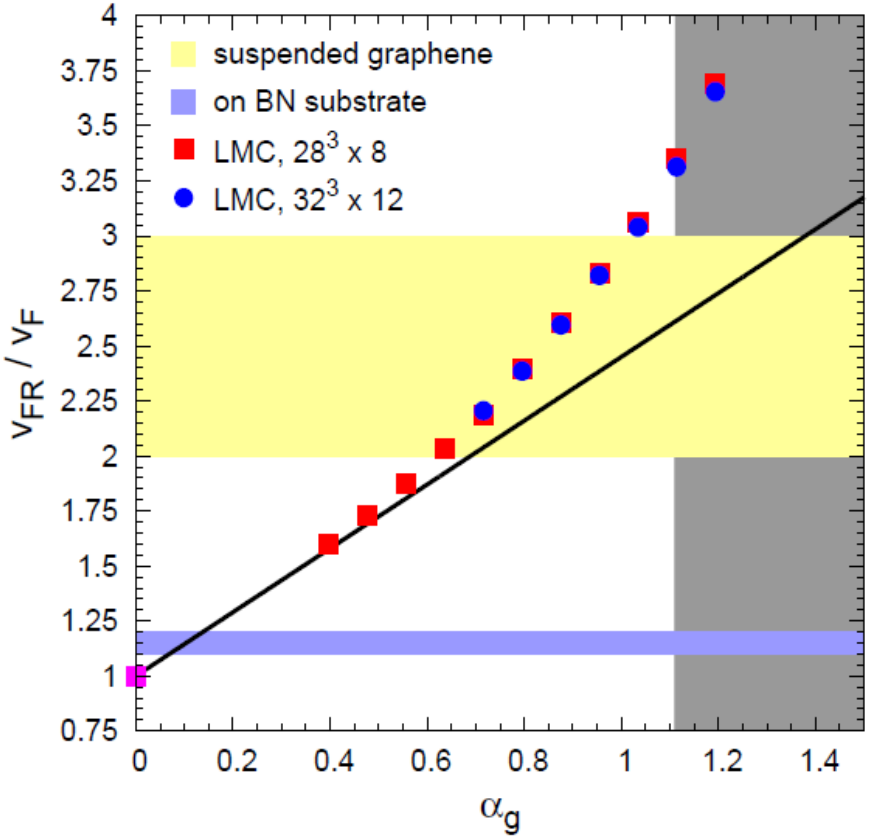
GW-DFT technique - «one-loop» electron self energy. Vertex corrections are neglected

$$\Sigma^{GW}(r, r', \omega) = \frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega' G(r, r', \omega - \omega') W(r, r', \omega'),$$



P. E. Trevisanutto et. al. PRL 101 (2008) 226405

Fermi Velocity renormalization obtained from measurements of lattice fermionic propagator (staggered fermions):



J. E. Drut, T. Lahde arXiv: 1304.1711 (talk at LATTICE 2013)

Hybrid Monte-Carlo simulations on honeycomb lattice (1)

We start from tight-binding hamiltonian:

$$\hat{H}_{tb} = -\kappa \sum_{<x,y>,s} \left(\hat{a}^{+}_{y,s}\hat{a}_{x,s} + \hat{a}^{+}_{x,s}\hat{a}_{y,s}\right) \qquad \kappa = 2.7eV$$

and add interaction with potentially arbitrary inter-electron potentials:

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

Hubbars-Stratonovich transformation is used to convert interaction to the form convenient for Monte-Carlo calculations:

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

Lattice partition function:

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

Hybrid Monte-Carlo simulations on honeycomb lattice (2): fermionic operator

Lattice fermionic action:

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

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

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

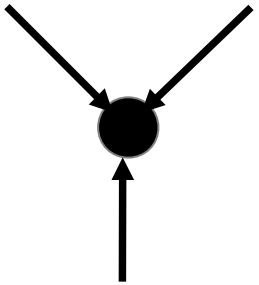
No sign problem!

Partition function:

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

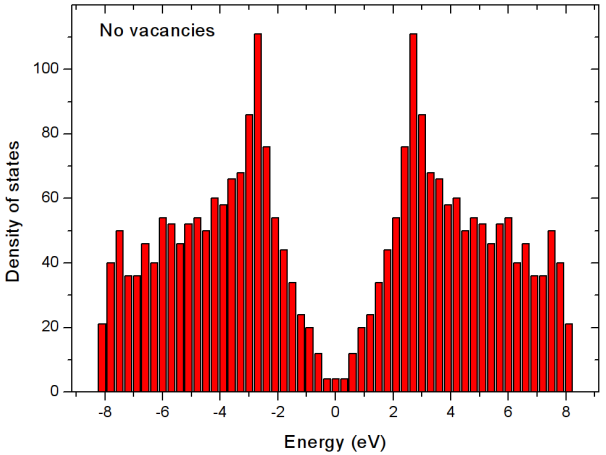
$$= \int \prod_{x,i} d\varphi^{(i)}_x \prod_{x,i} d\chi^{(i)*}_x d\chi^{(i)}_x e^{-S_{Hubbard}} e^{-\vec{\chi}^* \frac{1}{MM^+}\vec{\chi}}$$

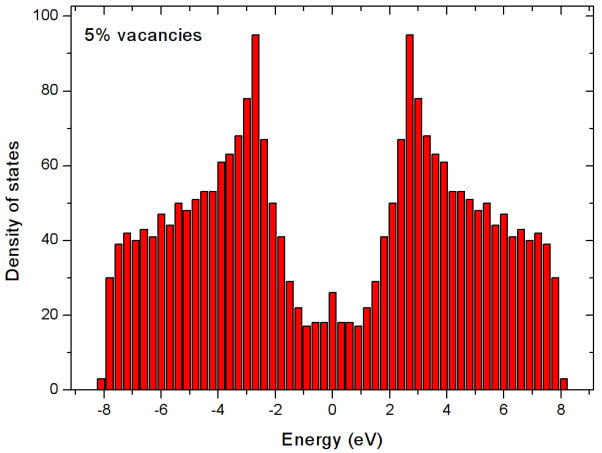
Graphene with vacancies



Hoppings are equal to zero for all links connecting vacant site with its neighbors. Charge of the site is also zero.

Approximately corresponds to Hydrogen adatoms.



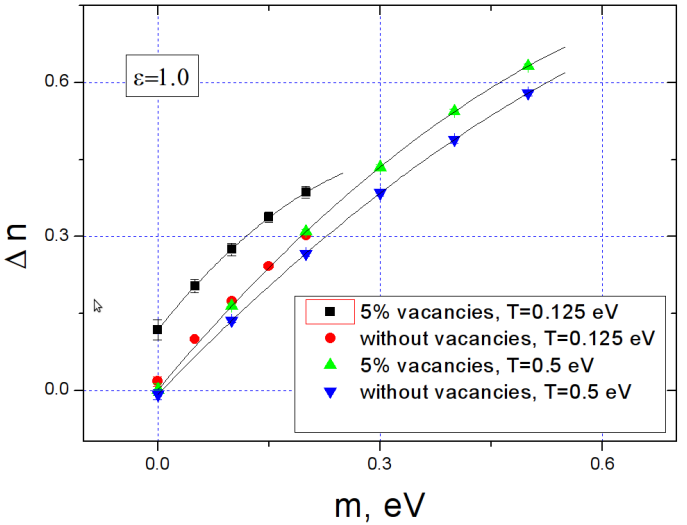


They work very similar to instantons in QFT because near-zero energy states appear in the vicinity of vacant sites. Increasing of the Density of states at Fermi-points will probably lead to instability with respect to formation of some condensate (mean field arguments, analogy to Banks-Casher relation in QCD).

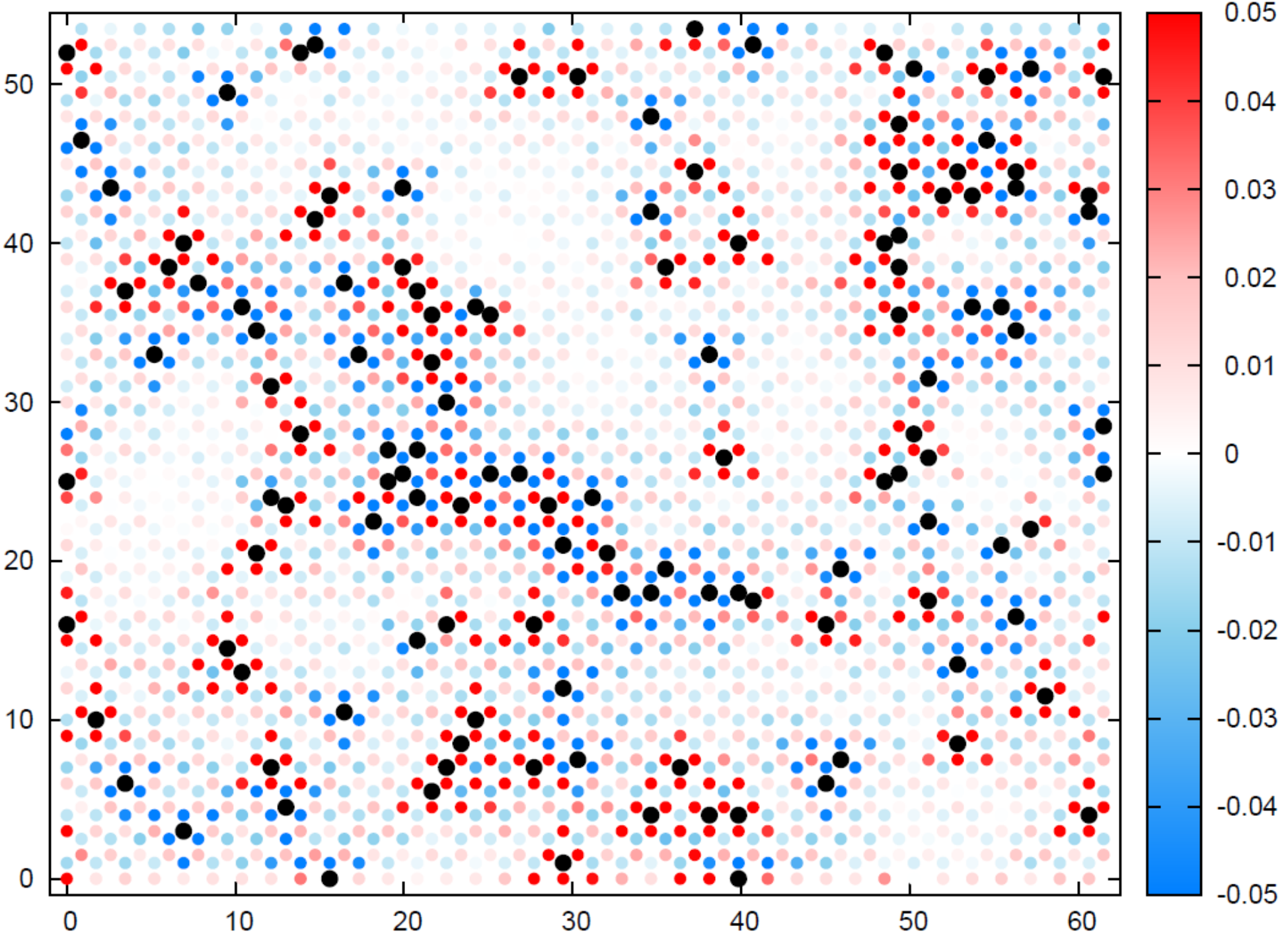
Antiferromagnetic condensate measurements at different temperatures without vacancies and in presence of 5% vacancies (suspended graphene):

Lattice size is 36 x 36 x 80.

Temperature suppresses the effect of vacancies.



Distribution of electron spin



Acceleration (1): Preconditioner for CG

Structure of fermionic operator:

$$M = \begin{pmatrix} 1 & -1+\delta H & & & & & & & & \\ & 1 & e^{i\varphi^{(0)}} & & & & & & & \\ & & 1 & -1+\delta H & & & & & & \\ & & & 1 & e^{i\varphi^{(1)}} & & & & & \\ & & & & \ddots & \ddots & & & & \\ & & & & & \ddots & \ddots & & & \\ & & & & & & 1 & e^{i\varphi^{(N_t-2)}} & & \\ & & & & & & & 1 & -1+\delta H & \\ -e^{i\varphi^{(N_t-1)}} & & & & & & & & 1 & \end{pmatrix}$$

Tight-binding Hamiltonian matrix

Diagonal matrix with Hubbard field exponents at the main diagonal

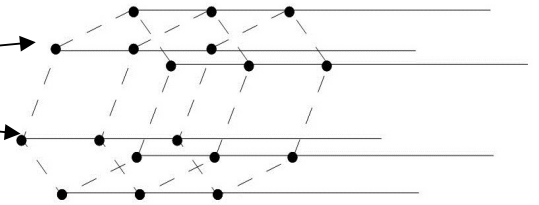
Preconditioner — operator with open boundary conditions in Euclidean time direction:

$$P = \begin{pmatrix} 1+\alpha & -1+\delta(\pm m) & & & & & & & & \\ & 1+\alpha & e^{i\varphi^{(0)}} & & & & & & & \\ & & 1+\alpha & -1+\delta(\pm m) & & & & & & \\ & & & 1+\alpha & e^{i\varphi^{(1)}} & & & & & \\ & & & & \ddots & \ddots & & & & \\ & & & & & \ddots & \ddots & & & \\ & & & & & & 1+\alpha & e^{i\varphi^{(N_t-2)}} & & \\ & & & & & & & 1+\alpha & -1+\delta(\pm m) & \\ & & & & & & & & 1+\alpha & \end{pmatrix}$$

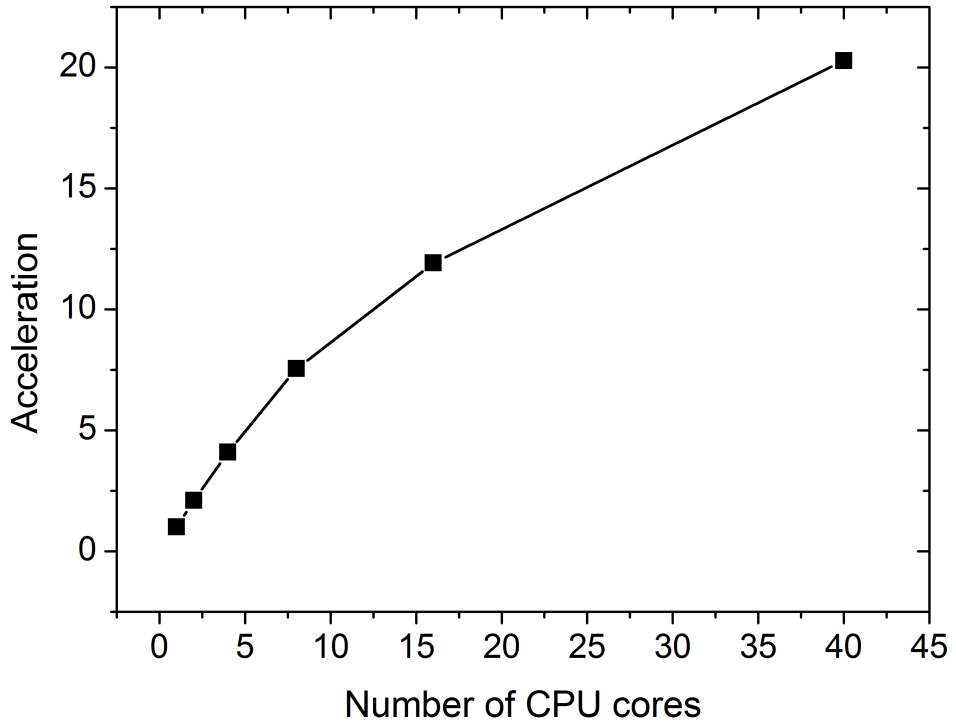
We need a regulator to avoid small eigenvalues

Hoppings inside time slices are turned off

The preconditioner equations can be solved separately for each set of sites with equal spatial indexes.
Number of iterations is ~3 times less in preconditioned CG.
Overall speedup is ~2.5 times.



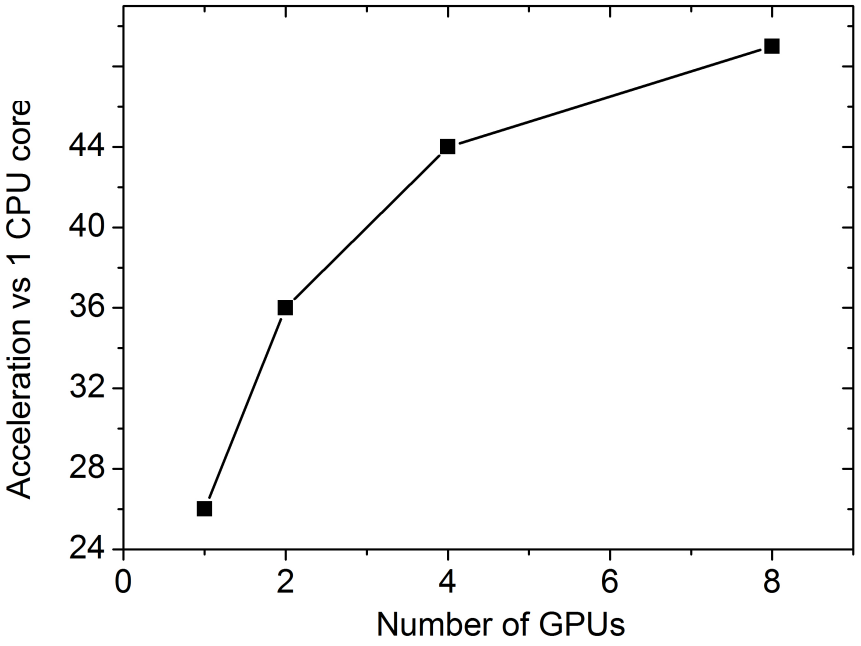
Acceleration (2): MPI-parallelisation and GPU



The simplest way to make a parallel algorithm is to divide lattice into several domains in Euclidean time direction.

1 GPU makes a speedup of ~20-25 times in comparison with 1 CPU core.

All the tests have been done for 36 x 36 x 80 lattice. CPU: Intel Xeon 5670
GPU: Nvidia M2070.

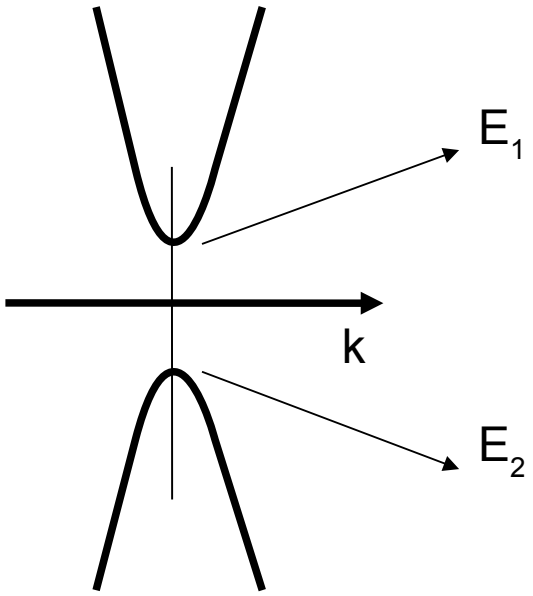


Mass gap calculation

We calculate the Euclidean Green function (simply inverse fermionic operator):

$$G_E(\vec{k},\tau) = \sum_{x,y} G_E(\vec{x},\vec{y},\tau) e^{i(\vec{x}-\vec{y})\vec{k}} \frac{1}{N_{xy}}$$

Sublatice structure of Green function after the Fourier transformaion:



$$G_E(\vec{k},\tau) = \begin{pmatrix} G_{AA}(\vec{k},\tau) & G_{AB}(\vec{k},\tau) \\ G_{BA}(\vec{k},\tau) & G_{BB}(\vec{k},\tau) \end{pmatrix}$$

Diagonal terms contain only two states (approximately):

$$G_{XX} \approx |C_1|^2 e^{-E_1(\vec{k})\tau} + |C_2|^2 e^{-E_2(\vec{k})\tau}$$

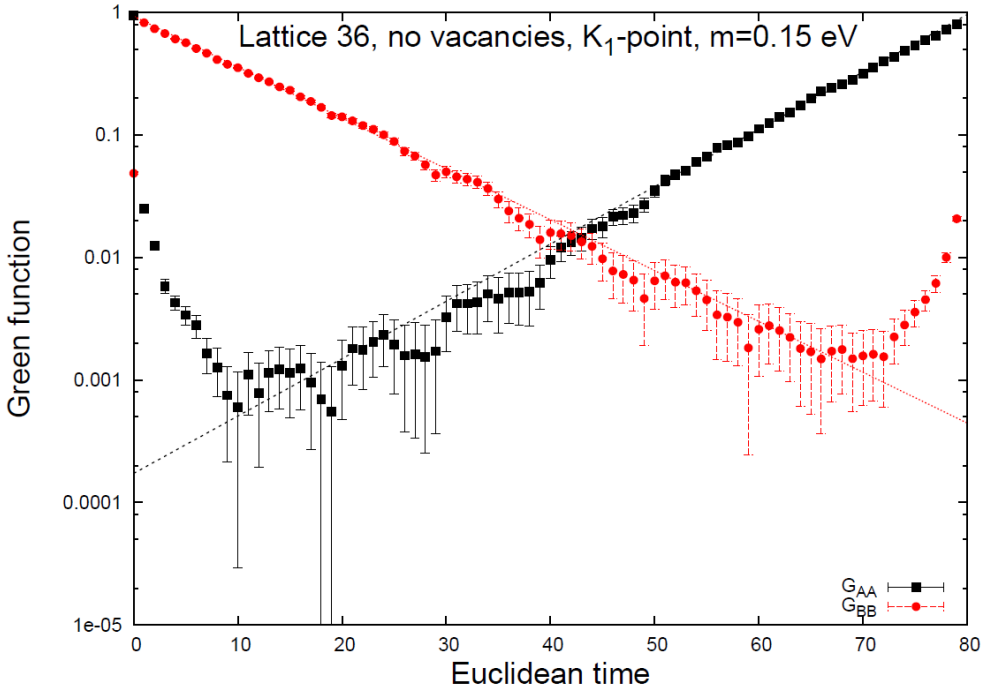
$$E_1(\vec{k}) > 0\,; \quad E_2(\vec{k}) < 0$$

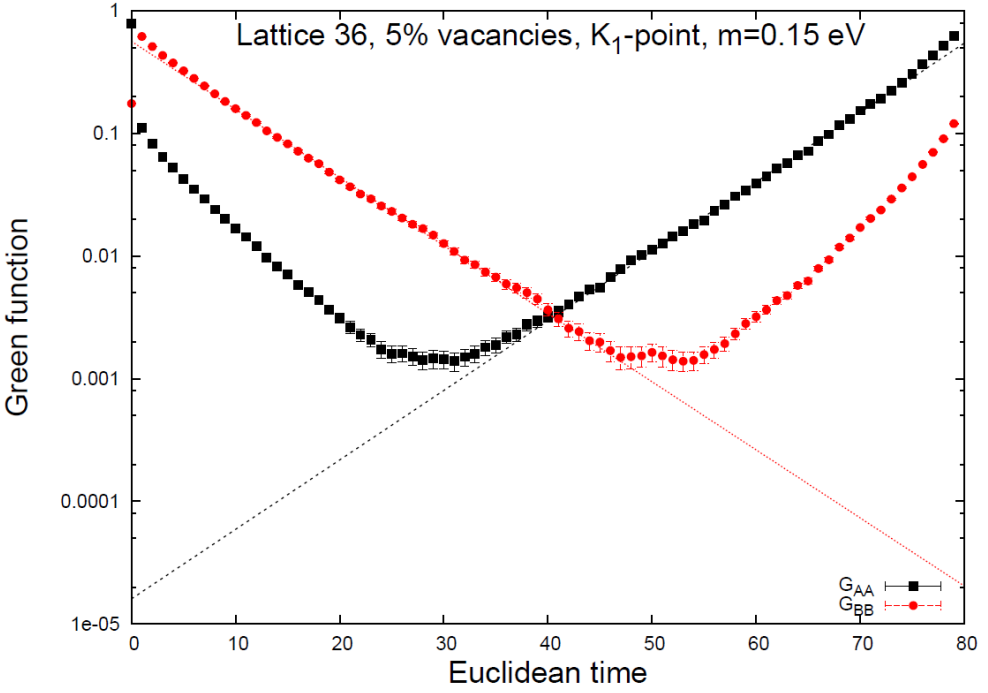
States at K-points are concentrated at one sublattice

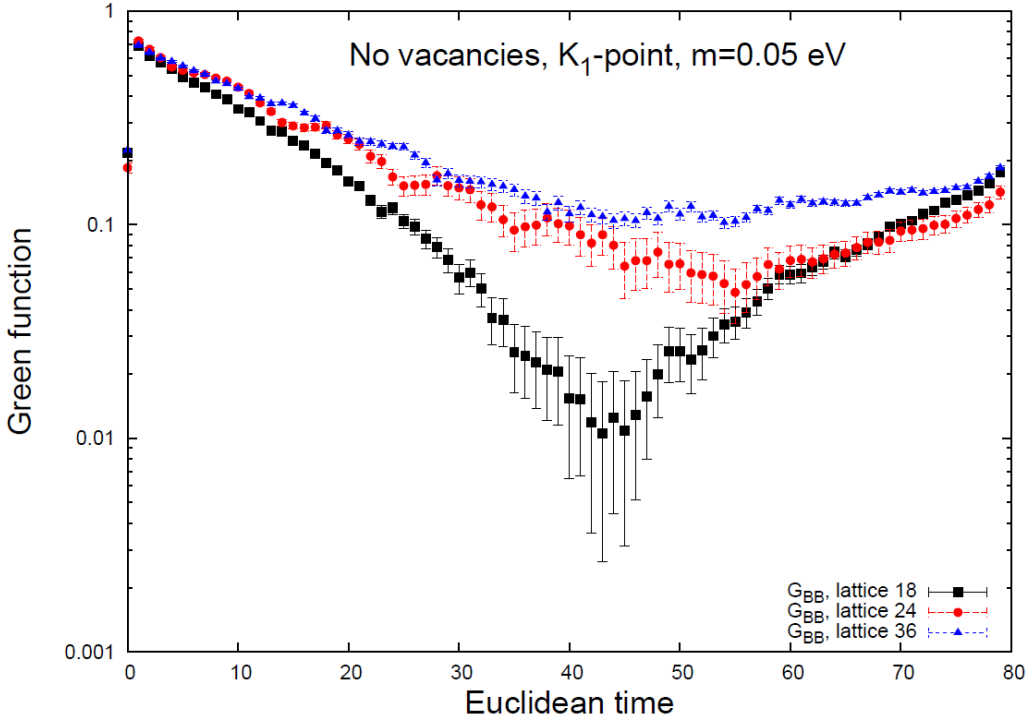
$$|C_1| \ll |C_2|$$

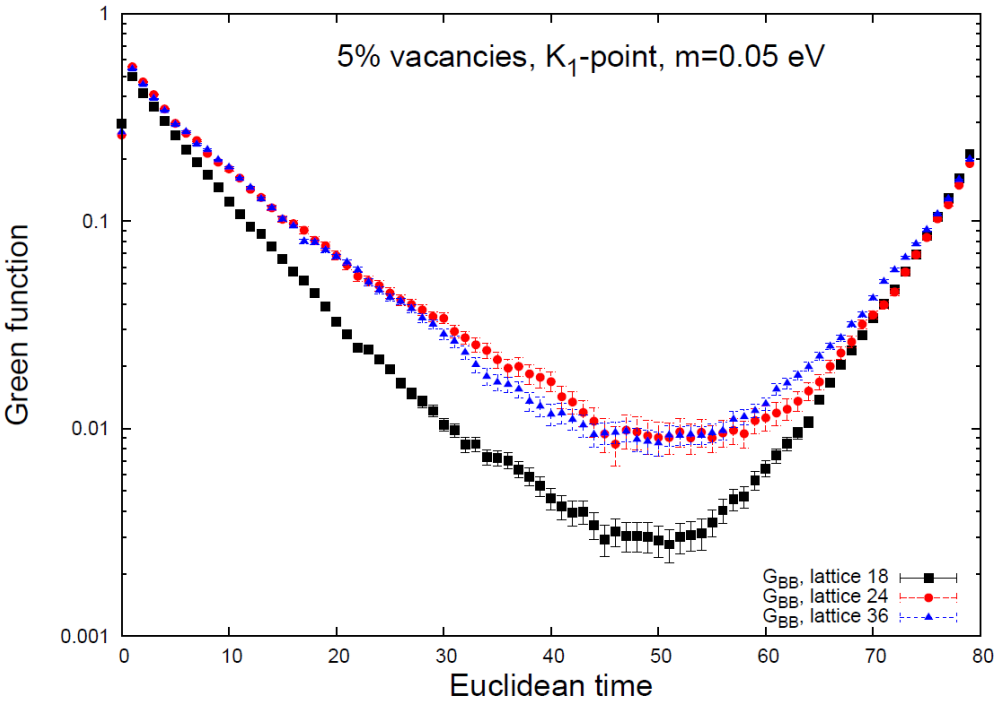
$$H(\vec{k}) = \begin{pmatrix} m & -\kappa f(\vec{k}) \\ -\kappa f^*(\vec{k}) & -m \end{pmatrix}$$

Green function calculations

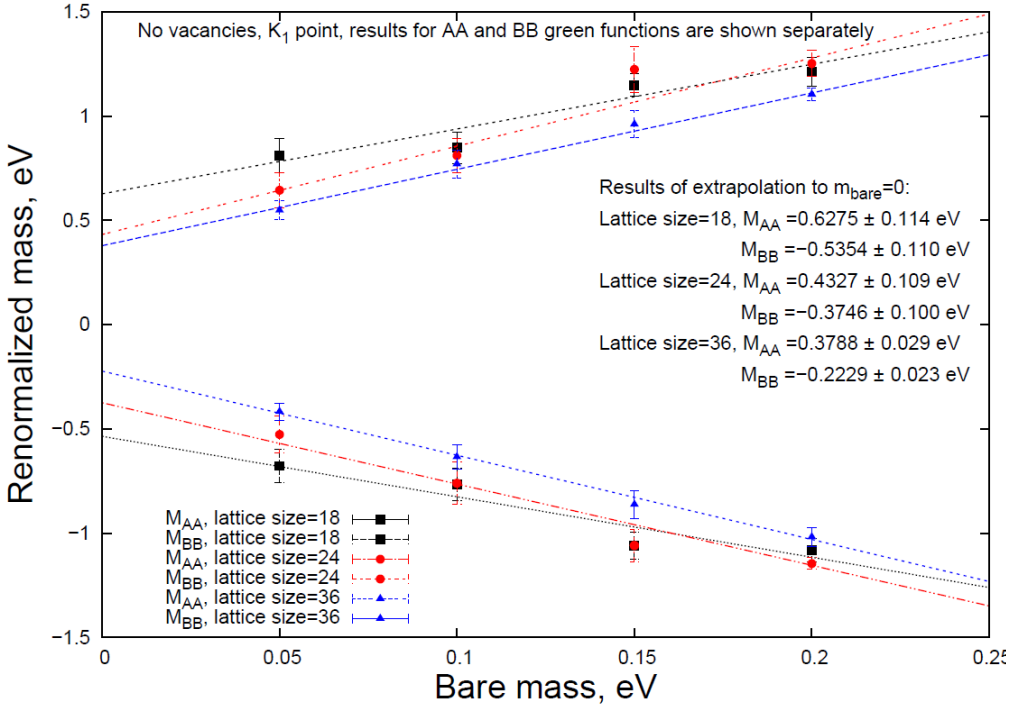


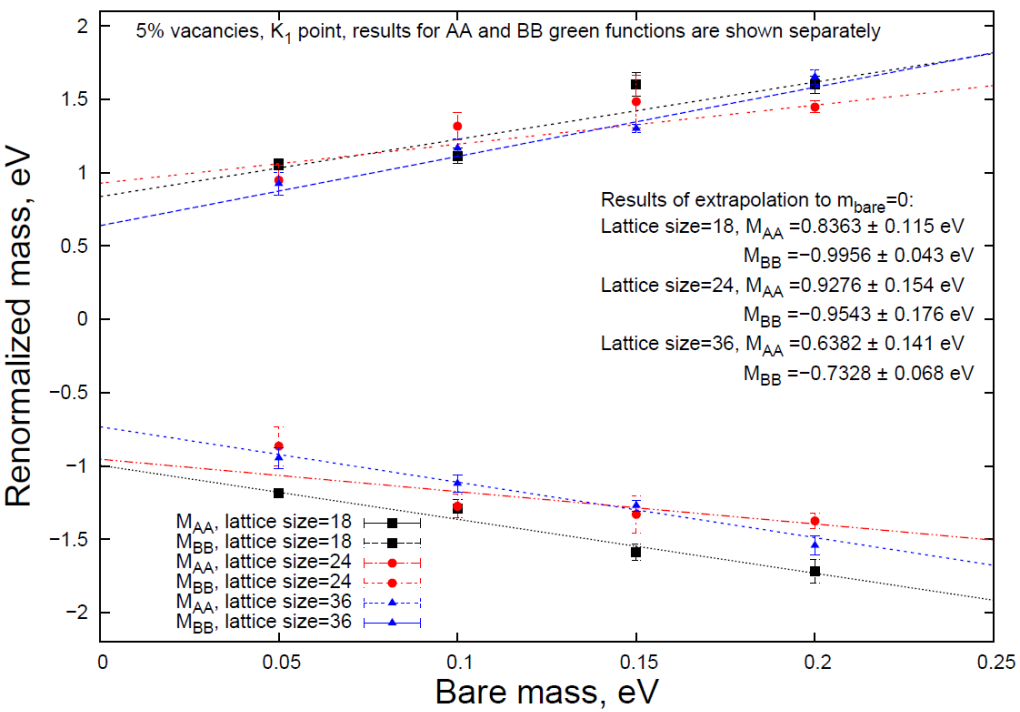


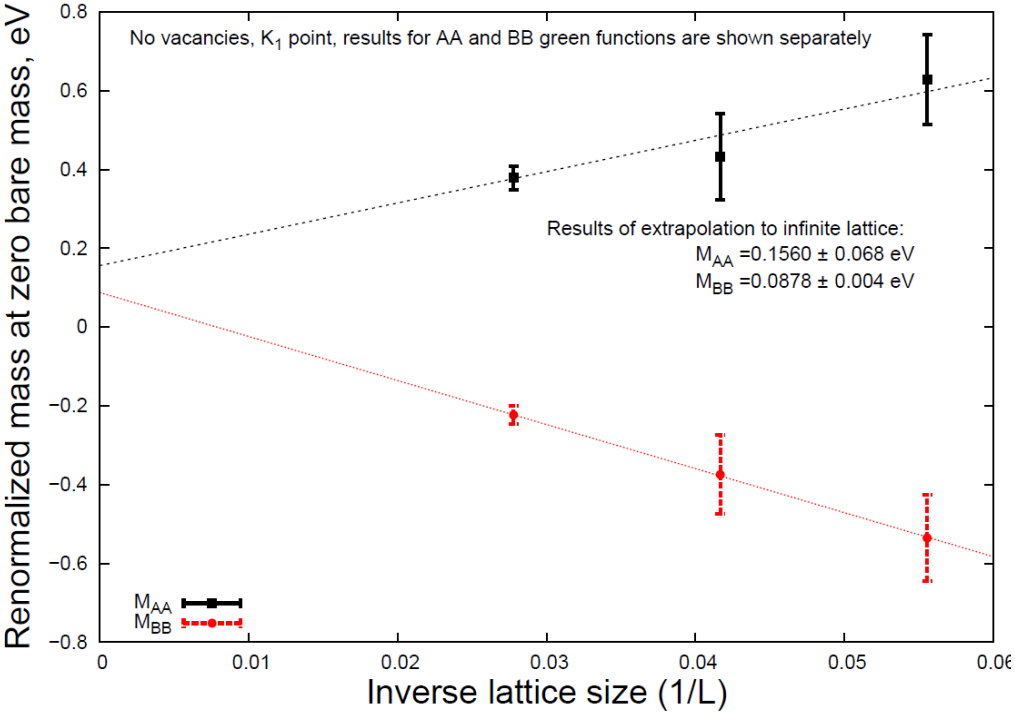


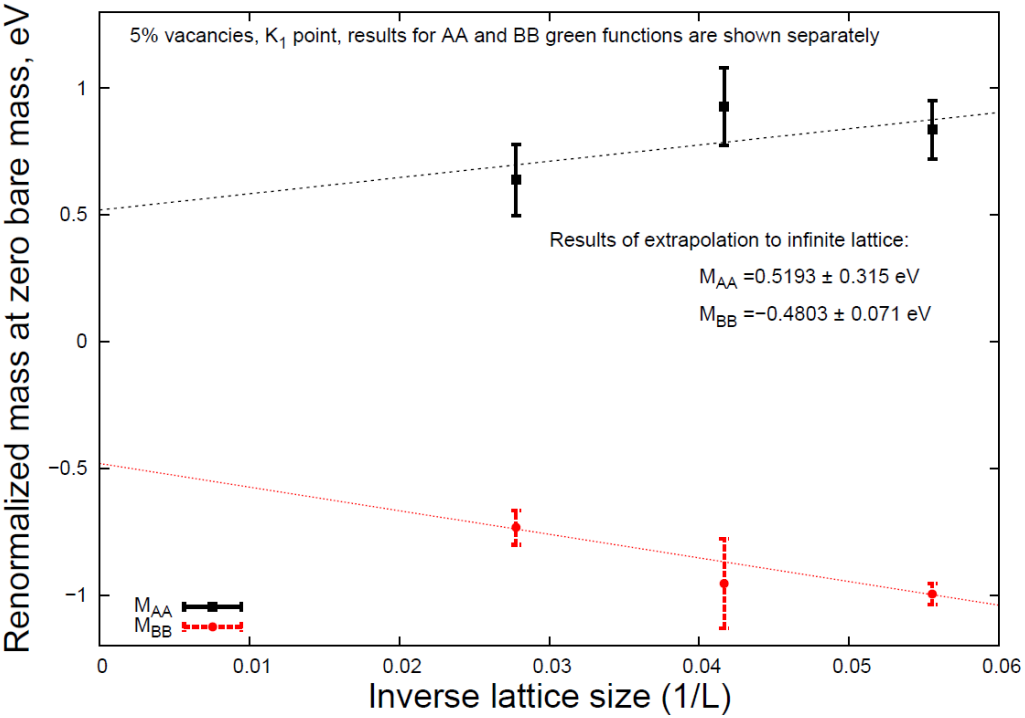


Mass gap calculation results









Conclusions:

1) In some circumstances (when we have well-defined tight binding model and avoid sign problem) Hybrid Monte-Carlo simulations can sufficiently improve our knowledge about effects of strong interaction in condensed matter physics.

2) As an example of such calculations we performed simulation of graphene in presence of vacancies. The results shows that their presence leads to the appearance of antiferromagnetic condensate and phase transition to an antiferromagnetic phase.

3) It seems that we still have some problems with calculation of mass gap. Correct result (zero mass gap in suspended graphene) can be obtained only in the limit of infinitely large lattice.