Hexagonal lattice model of the AA-stacked bilayer graphene

A. A. Nikolaev[1]*, **M. V. Ulybyshev**[2]

[1]Far Eastern Federal University; [2]Regensburg University, ITEP and Moscow State University

*nikolaev.aa@dvfu.ru

Abstract

Tight-binding model of the AA-stacked bilayer graphene with screened electron-electron interactions has been studied using the Hybrid Monte Carlo simulations on the original double-layer hexagonal lattice. Instantaneous screened Coulomb potential is taken into account using Hubbard-Stratonovich transformation. G-type antiferromagnetic ordering has been studied and the phase transition with spontaneous generation of the mass gap has been observed. Dependence of the antiferromagnetic condensate on the on-site electron-electron interaction is examined.

Monolayer graphene and bilayer graphene

Monolayer graphene is represented by a single sheet of carbon atoms, which form hexagonal lattice. Each carbon atom has 4 valence electrons, 3 of them form σ-bonds and the last remains on π-orbital.

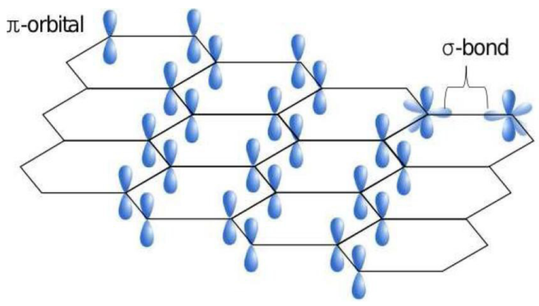

Figure 1: *Atomic structure of monolayer graphene. Electrons on π-orbitals are oriented perpendicular to the graphene plane.*

Bilayer graphene is represented by two graphene sheets, stacked upon each other.

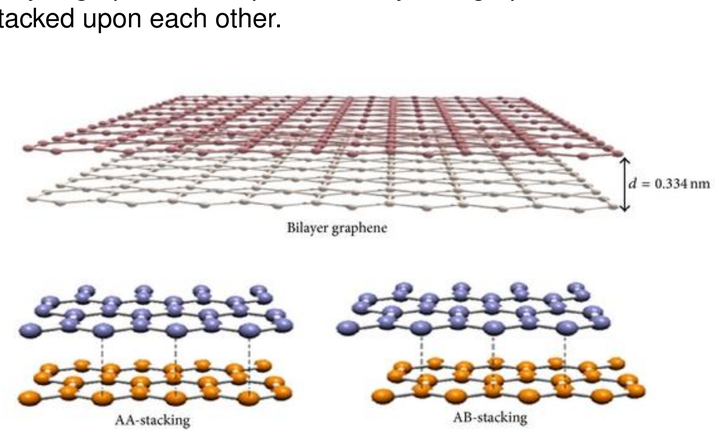

Figure 2: *Two common types of bilayer graphene. Energy spectrum of electrons and transport properties depends heavily on the way of stacking.*

We concentrate on the AA-stacked bilayer graphene (AA-BLG).

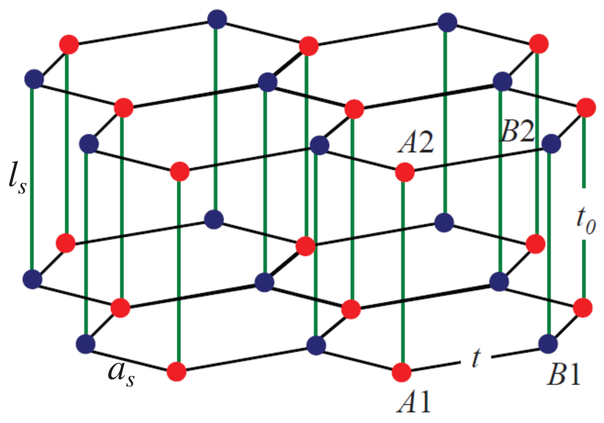

Figure 3: *Atomic structure of the elementary cell of AA-BLG ($a_s = 1.42$ A, $l_s = 3.3$ A).*

Tight-binding Hamiltonian for electrons in the AA-BLG may be written as follows:

$$\hat{H}_{tb} = -t\sum_{i=1}^{2}\sum_{<X_i,Y_i>}\sum_{\sigma=\uparrow,\downarrow}\hat{a}^{+}_{X_i\sigma}\hat{a}_{Y_i\sigma} - -t_0\sum_{X}\sum_{\sigma=\uparrow,\downarrow}\hat{a}^{+}_{X_1\sigma}\hat{a}_{X_2\sigma} + h.c.,$$

where $\hat{a}^{+}_{X_i\sigma}$ and $\hat{a}_{X_i\sigma}$ are creation and annihilation operators for the electron with spin σ at the site X on the layer i respectively, $t = 2.57$eV represents nearest-neighbour hopping inside one layer and $t_0 = 0.36$eV — between layers (values of hoppings are taken from [1]).

Energy spectrum of such system has the following form:

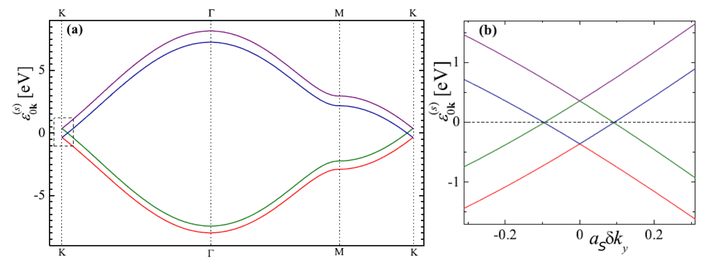

Figure 4: *Energy spectrum of AA-BLG from tight-binding Hamiltonian.*

Near the Dirac points:

$$\epsilon = v_F|\mathbf{k}|,$$

where $v_F = \frac{3}{2}ta \approx \frac{1}{315} \Rightarrow$

- coupling constant $\alpha = \frac{e^2}{v_F} \approx 2.3$, in AA-BLG we have **electrodynamics with a strong interaction**
- magnetic and retardation effects can be neglected, **only Coulomb interaction may be considered**

Interaction potentials: screened Coulomb inside the graphene layer, usual Coulomb between the layers.

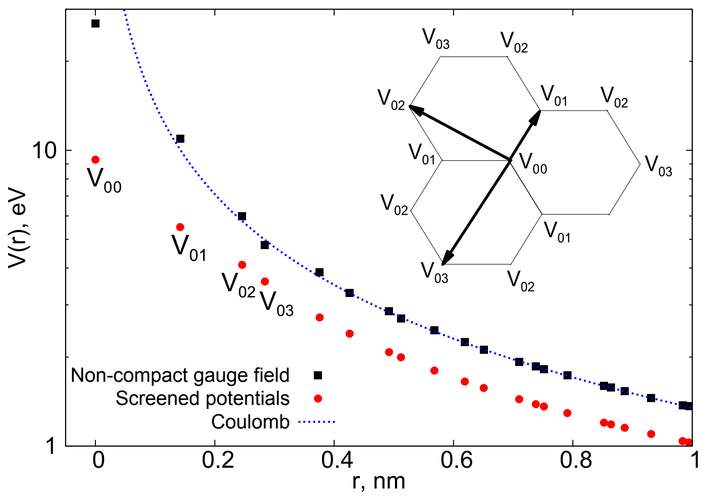

Figure 5: *Electron-electron interaction potential inside one graphene layer. For detailed dicsussion about screening by σ-electrons see [2].*

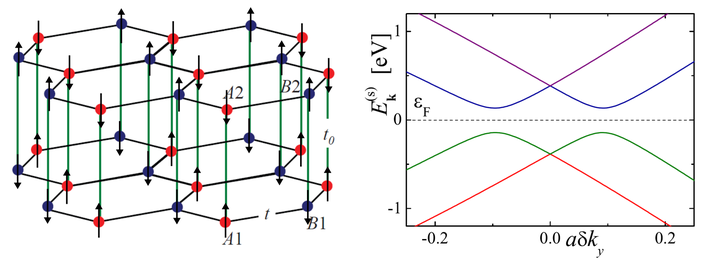

Figure 6: *There are arguments from mean-field theory, that Coulomb interaction in the AA-BLG may open the energy gap and lead to formation of G-type AFM condensate [3]*

Lattice formulation

We start from the **Hamiltonian formulation** of partition function. Hamiltinian is formulated in terms of electrons and holes:

$$\hat{H} = \hat{H}_{tb} + \hat{H}_{stag.} + \hat{H}_{int.}$$

$$\hat{H}_{tb} = -t\sum_{i=1}^{2}\sum_{<X_i,Y_i>}(\hat{a}^{+}_{X_i}\hat{a}_{Y_i} + \hat{b}^{+}_{X_i}\hat{b}_{Y_i}) - - t_0\sum_{X}(\hat{a}^{+}_{X_1}\hat{a}_{X_2} + \hat{b}^{+}_{X_1}\hat{b}_{X_2}) + h.c.$$

$$\hat{H}_{st.} = \sum_{i=1}^{2}\sum_{X,Y}\pm m\hat{a}^{+}_{X_i}\hat{a}_{Y_i} \pm m\hat{b}^{+}_{X_i}\hat{b}_{Y_i},$$

where the sign before m in the $\hat{H}_{st.}$ are chosen according to the left part of Fig. 6. Electron-electron interaction are added by

$$\hat{H}_{int.} = \frac{1}{2}\sum_{i,j=1}^{2}\sum_{X,Y}\hat{q}_{X_i}V^{ij}_{XY}\hat{q}_{Y_j},$$

where $\hat{q}_{X_i} = \hat{a}^{+}_{X_i}\hat{a}_{X_i} - \hat{b}^{+}_{X_i}\hat{b}_{X_i}$ and V^{ij}_{XY} is the matrix of potentials.

Exponentials in partition function are splitted as follows:

$$Z = Tr\left(e^{-\beta\hat{H}}\right) = Tr\left(e^{-\Delta\tau(\hat{H}_{tb}+\hat{H}_{stag.}+\hat{H}_{int.})}\right)^{N_t} = = Tr\left(e^{-\Delta\tau(\hat{H}_{tb}+\hat{H}_{st.})}e^{-\Delta\tau\hat{H}_{int.}}e^{-\Delta\tau(\hat{H}_{tb}+\hat{H}_{st.})}\dots\right) + O(\Delta\tau^2)$$

Important feature: there are now $2N_t$ time layers due to such splitting, **only even time layers are physical**.

To deal with $e^{-\Delta\tau\hat{H}_{int.}}$ we perform Hubbard-Stratonovich transformation [4]:

$$e^{-\frac{\Delta\tau}{2}\sum\limits_{X,Y}\hat{q}_X V_{XY}\hat{q}_Y} = \int\mathcal{D}\varphi e^{-\frac{1}{2\Delta\tau}\sum\limits_{X,Y}\varphi_X V^{-1}_{XY}\varphi_Y - i\sum\limits_X\varphi_X\hat{q}_X}$$

Finally we arrive at the following expression:

$$Z = \int\mathcal{D}\varphi\mathcal{D}\overline{\eta}\mathcal{D}\eta\mathcal{D}\overline{\chi}\mathcal{D}\chi e^{-\overline{\eta}M\eta - \overline{\chi}M^{+}\chi - \frac{1}{2\Delta\tau}\varphi^T\hat{V}^{-1}\varphi} = \int\mathcal{D}\varphi det(M^{+}M)e^{-\frac{1}{2\Delta\tau}\varphi^T\hat{V}^{-1}\varphi}$$

Fermionic determinant is positive!

The observable: AFM condensate. Electron density operators:

$$\hat{n}_{iA\uparrow} = \frac{1}{N_{subl.}}\sum_{X\in A}\hat{a}^{+}_{X_A,i\uparrow}\hat{a}_{X_A,i\uparrow}$$

$$\hat{n}_{iB\downarrow} = \frac{1}{N_{subl.}}\sum_{X\in B}\hat{a}^{+}_{X_B,i\downarrow}\hat{a}_{X_B,i\downarrow}$$

$$\Delta n = \langle\hat{n}_{1A\uparrow}\rangle - \langle\hat{n}_{2A\uparrow}\rangle = \langle\hat{n}_{1B\downarrow}\rangle - \langle\hat{n}_{2B\downarrow}\rangle$$

In terms of inverse Dirac operator:

$$\langle\Delta n\rangle = \frac{1}{N_\tau N_{subl.}}\sum_\tau\left\langle\sum_{X\in A}\left(\hat{M}^{-1}_{X2X2} - \hat{M}^{-1}_{X1X1}\right)\right\rangle = \frac{1}{N_\tau N_{subl.}}\sum_\tau\left\langle\sum_{X\in B}\left(\hat{M}^{-1}_{X1X1} - \hat{M}^{-1}_{X2X2}\right)\right\rangle$$

Numerical results

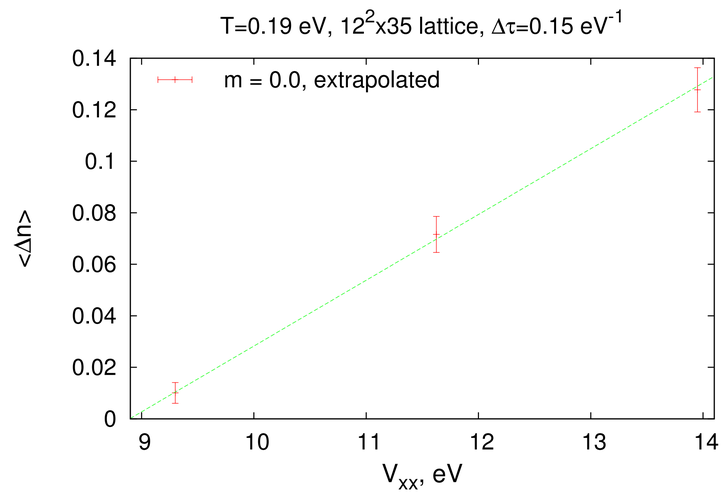

Figure 7: *The dependence of the AFM condensate on the on-site interaction potential V_{xx} at fixed temperature. AFM condensate vanishes at the value (8.89 $\pm$ 0.33) eV.*

Here we have **disagreement with MF result**: $\Delta n \approx 0.5$ at $V_{xx} = 8.9$ eV [3].

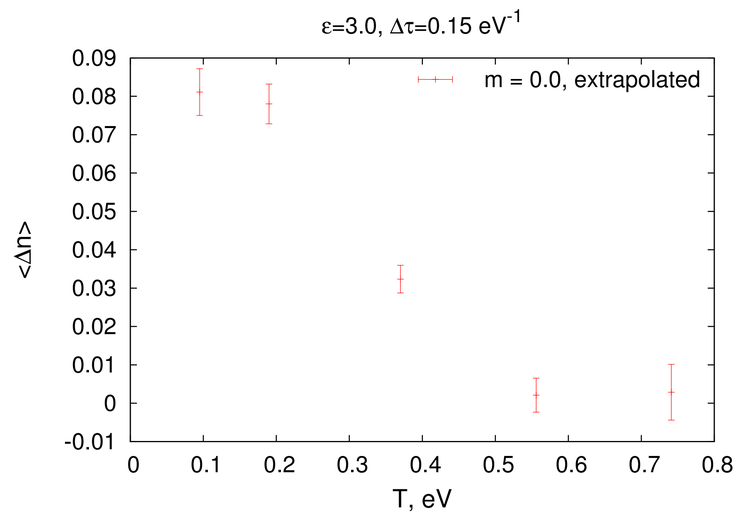

Figure 8: *The dependence of the AFM condensate on temperature, measured on lattices with different temporal sizes. All potentials, except V_{xx}, were rescaled by the factor of $\epsilon = 3.0$: $V^{ij}_{XY} \to V^{ij}_{XY}/3.0$.*

Conclusions

- Original hexagonal lattice model for AA-bilayer graphene with long-range Coulumb interaction was studied.
- Formation of the AFM condensate was observed and its dependence on the on-site electron-electron interaction was examined.

References

[1] J.-C. Charlier, J.-P. Michenaud, and X. Gonze, Phys. Rev. B **46**, 4531 (1992).

[2] M. V. Ulybyshev, P. V. Buividovich, M. I. Katsnelson, M. I. Polikarpov, Phys. Rev. Lett. **111**, 056801 (2013).

[3] A. L. Rakhmanov, A. V. Rozhkov, A. O. Sboychakov, and Franco Nori, Phys. Rev. Lett. **109**, 206801 (2012).

[4] R. C. Brower, C. Rebbi, and D. Schaich, *PoS(Lattice 2011)056*.