Monte-Carlo study of the phase transition in the AA-stacked bilayer graphene

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Outline

- Introduction
- Tight-binding Hamiltonian and energy spectrum
- Lattice field model
- Numerical results for the AFM condensate

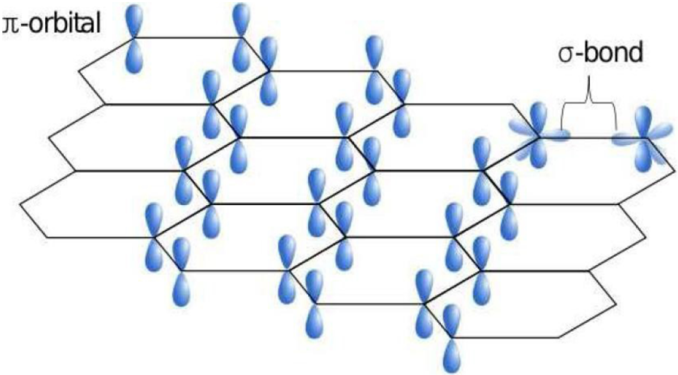
Historical remarks

2004 — first experimental observation of graphene (Science 306 (5696): 666-669)

2010 — the Nobel Prize was awarded to Andre Geim and Konstantin Novoselov

Graphene: atomic structure

Each carbon atom has 4 valence electrons: 3 of them form σ-bonds and the last remains on π-orbital.



Why do we need lattice calculations for AA-bilayer graphene?

Methodological interest:

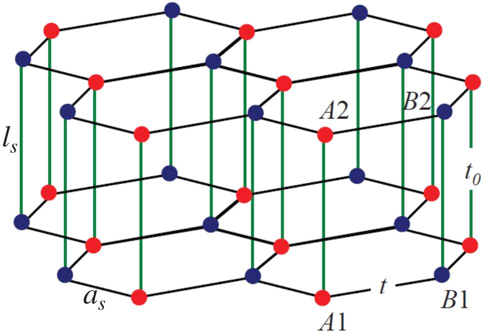
- We can compare LFT results with the Condensed Matter Physics predictions
- Intermediate step to the lattice models of multilayer graphene
- No non-perturbative calculations have been performed yet
- Symmetrical energy spectrum $\Rightarrow$ no sign problem
- Possibilities to study finite temperature effects

Why not to try?

Atomic structure and tight-binding Hamiltonian

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

$$\{\hat{a}_{X_i\sigma}, \hat{a}^{+}_{Y_j\sigma'}\} = \delta_{X_i Y_j}\delta_{\sigma\sigma'} \qquad \{\hat{a}_{X_i\sigma}, \hat{a}_{Y_j\sigma'}\} = 0 \qquad \{\hat{a}^{+}_{X_i\sigma}, \hat{a}^{+}_{Y_j\sigma'}\} = 0$$



$a_s = 1.42$ A
$l_s = 3.3$ A

$t = 2.57$ eV
$t_0 = 0.36$ eV

Tight-binding Hamiltonian

In momentum representation:

$$\hat{H}^{tb}_{\mathbf{k}} = - \begin{pmatrix} 0 & t_0 & t|f_{\mathbf{k}}| & 0 \\ t_0 & 0 & 0 & t|f_{\mathbf{k}}| \\ t|f_{\mathbf{k}}| & 0 & 0 & t_0 \\ 0 & t|f_{\mathbf{k}}| & t_0 & 0 \end{pmatrix} = -t_0 \hat{\tau}_x \otimes 1 - t 1 \otimes \hat{\sigma}_x |f_{\mathbf{k}}|,$$

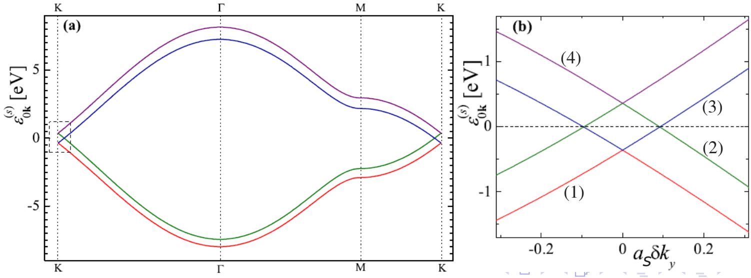
where $f_{\mathbf{k}} = 1 + 2e^{i\frac{3k_x a}{2}} cos(\frac{k_y a\sqrt{3}}{2})$, $\hat{\tau}_x$ and $\hat{\sigma}_x$ — Pauli matrices acting in layer space and sublattice space respectively.
Symmetries of the Hamiltonian:

$$[\hat{\sigma}_x, \hat{H}^{tb}_{\mathbf{k}}] = 0 \Rightarrow \sigma = \pm 1 \qquad [\hat{\tau}_x, \hat{H}^{tb}_{\mathbf{k}}] = 0 \Rightarrow \tau = \pm 1$$

Energy bands without interaction

$$\epsilon^{(1)}_{0\mathbf{k}} = -t_0 - t|f_{\mathbf{k}}|, \quad \sigma = 1, \quad \tau = 1$$
$$\epsilon^{(2)}_{0\mathbf{k}} = t_0 - t|f_{\mathbf{k}}|, \quad \sigma = 1, \quad \tau = -1$$
$$\epsilon^{(3)}_{0\mathbf{k}} = -t_0 + t|f_{\mathbf{k}}|, \quad \sigma = -1, \quad \tau = 1$$
$$\epsilon^{(4)}_{0\mathbf{k}} = t_0 + t|f_{\mathbf{k}}|, \quad \sigma = -1, \quad \tau = -1$$

where $f_{\mathbf{k}} = 1 + 2e^{i\frac{3k_x a}{2}} cos(\frac{k_y a\sqrt{3}}{2})$.

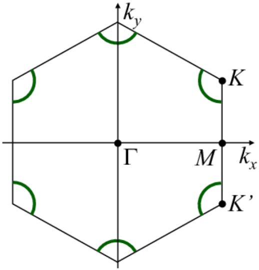


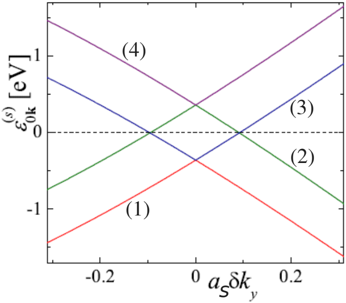
E(k) dispersion relation at low energies

$\epsilon_F = 0 \Rightarrow \epsilon^{(2)}_{0\mathbf{k}}$ and $\epsilon^{(3)}_{0\mathbf{k}}$ form Fermi arcs with the radius $k_r = \frac{2t_0}{3ta}$.

Near the Dirac points: $\epsilon = v_F|\mathbf{k}|$, where $v_F = \frac{3}{2}ta \approx \frac{1}{315} \Rightarrow$

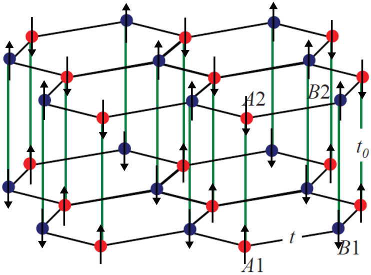
$$\alpha = \frac{e^2}{v_F} \approx 2.3$$





G-type AFM ordering

Fermi surfaces are degenerate and have different values of σ and τ $\Rightarrow$ G-type AFM ordering will break both sublattice and interlayer symmetries and induce energy gap



Electron densities:

$$n_{1A\uparrow} = n_{2B\uparrow} = n_{2A\downarrow} = n_{1B\downarrow} = \frac{1 + \Delta n}{2}$$

$$n_{1A\downarrow} = n_{2B\downarrow} = n_{2A\uparrow} = n_{1B\uparrow} = \frac{1 - \Delta n}{2}$$

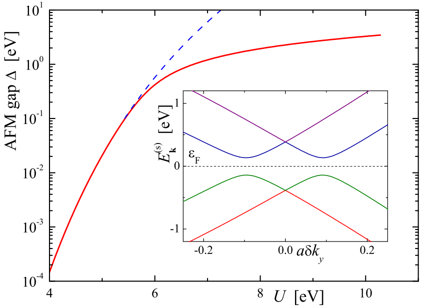
Charge conservation: $n_{iA\uparrow} + n_{iA\downarrow} = n_{iB\uparrow} + n_{iB\downarrow} = 1$

AFM condensate: $\Delta n = n_{1A\uparrow} - n_{2A\uparrow} = n_{1B\downarrow} - n_{2B\downarrow}$

On-site Coulomb interaction

G-type AFM ordering may be formed due to the on-site electron-electron interaction[1]:

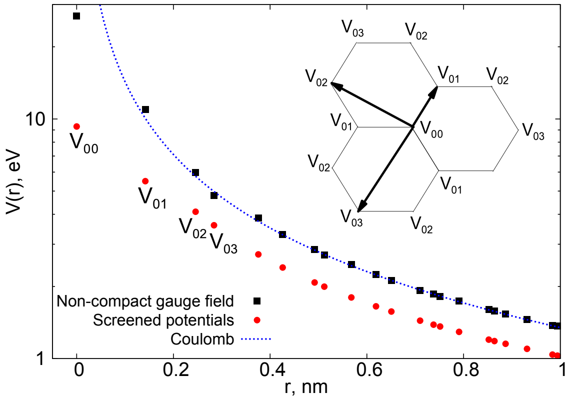
$$\hat{H}_{int.} = \frac{U}{2}\sum_{i,j=1}^{2}\sum_{X\in A}\sum_{\sigma=\downarrow,\uparrow}\hat{n}_{X_i\sigma}\hat{n}_{X_i-\sigma} + \frac{U}{2}\sum_{i,j=1}^{2}\sum_{X\in B}\sum_{\sigma=\downarrow,\uparrow}\hat{n}_{X_i\sigma}\hat{n}_{X_i-\sigma}$$



[1] A.L. Rakhmanov, A.V. Rozhkov, A.O. Sboychakov and F. Nori, PRL 109, 206801 (2012)

Our model: realistic inter-electron Coulomb potentials

We employ long-range Coulomb interaction and take into account screening by σ-orbitals within one layer[2]:



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

Creation and annihilation operators

Vacuum state: all spins are down.
It is convenient to introduce electrons:

$$\hat{a}^{+}_{X,i} = \hat{a}^{+}_{X,i\uparrow}$$

and holes:

$$\hat{b}^{+}_{X,i} = \begin{cases} \hat{a}_{X,i\downarrow}, & \text{layer 1, sublattice A} \\ -\hat{a}_{X,i\downarrow}, & \text{layer 1, sublattice B} \\ -\hat{a}_{X,i\downarrow}, & \text{layer 2, sublattice A} \\ \hat{a}_{X,i\downarrow}, & \text{layer 2, sublattice B} \end{cases}$$

Charge operator: $\hat{q}_{X_i} = \hat{a}^{+}_{X_i\uparrow}\hat{a}_{X_i\uparrow} + \hat{a}^{+}_{X_i\downarrow}\hat{a}_{X_i\downarrow} - 1 = \hat{a}^{+}_{X_i}\hat{a}_{X_i} - \hat{b}^{+}_{X_i}\hat{b}_{X_i}$.

Tight-binding Hamiltionain with interaction

Hamiltonian can now be formulated in terms of electrons and holes:

$$\begin{aligned}
\hat{H} &= \hat{H}_{tb} + \hat{H}_{stag.} + \hat{H}_{int.} \\
\hat{H}_{tb} &= -t \sum_{i=1}^{2} \sum_{<X_i, Y_i>} (\hat{a}^{+}_{X_i} \hat{a}_{Y_i} + \hat{b}^{+}_{X_i} \hat{b}_{Y_i}) - t_0 \sum_{X} (\hat{a}^{+}_{X_1} \hat{a}_{X_2} + \hat{b}^{+}_{X_1} \hat{b}_{X_2}) + h.c. \\
\hat{H}_{stag.} &= m \sum_{i=1}^{2} \sum_{X,Y} \left[(-1)^{i+1} \delta_{X_A Y_A} + (-1)^{i} \delta_{X_B Y_B} \right] (\hat{a}^{+}_{X_i} \hat{a}_{Y_i} + \hat{b}^{+}_{X_i} \hat{b}_{Y_i}) \\
\hat{H}_{int.} &= \frac{1}{2} \sum_{i,j=1}^{2} \sum_{X,Y} \hat{q}_{X_i} V^{ij}_{XY} \hat{q}_{Y_j}, \quad \text{where} \quad \hat{q}_{X_i} = \hat{a}^{+}_{X_i} \hat{a}_{X_i} - \hat{b}^{+}_{X_i} \hat{b}_{X_i}
\end{aligned}$$

Partition function: $Z = Tr\left(e^{-\beta \hat{H}}\right), \quad \beta = \frac{1}{T}.$

Partition function calculation

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

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

Standard method — inserting Grassmannian coherent states:

$$\left|\eta^\tau\chi^\tau\right\rangle = e^{\sum\limits_{Xi}\eta^\tau_{Xi}\left(\hat{a}^+_{Xi}\right)^\tau+\sum\limits_{Xi}\chi^\tau_{Xi}\left(\hat{b}^+_{Xi}\right)^\tau}\left|0\right\rangle$$

$$I = \int\mathcal{D}\overline{\eta}\mathcal{D}\eta\mathcal{D}\overline{\chi}\mathcal{D}\chi e^{-\sum\limits_{Xi}\overline{\chi}^\tau_{Xi}\chi^\tau_{Xi}-\sum\limits_{Xi}\overline{\eta}^\tau_{Xi}\eta^\tau_{Xi}}\left|\eta^\tau\chi^\tau\right\rangle\left\langle\eta^\tau\chi^\tau\right|$$

$$\left\langle\eta\right| e^{\sum\limits_{X,Y}\hat{a}^+_X A_{XY}\hat{a}_Y}\left|\eta'\right\rangle = e^{\sum\limits_{X,Y}\overline{\eta}_X(e^A)_{XY}\eta'_Y}$$

Important feature: now we have $2N_t$ time layers, only even time layers are physical.

Partition function

It is convenient to perform Hubbard-Stratonovich transformation[a]:

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

Finally we arrive at the following expression:

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

Fermionic determinant is positive!

An observable: $\langle O\rangle = \frac{1}{Z}Tr\left(\hat{O}e^{-\beta\hat{H}}\right)$

[a] PoS LAT2011, 056 (2012), ArXiv:1204.5424

Observable: AFM condensate

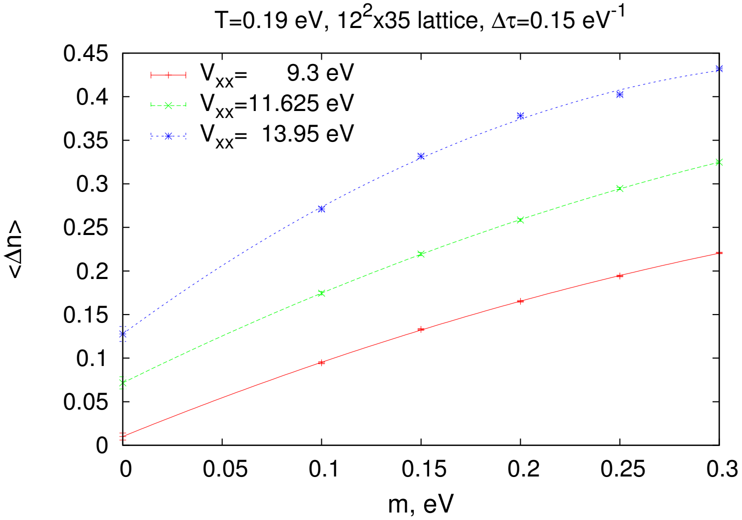
Electron density operators:

$$\begin{aligned}
\hat{n}_{iA\uparrow} &= \frac{1}{N_{subl.}} \sum_{X\in A} \hat{a}^{+}_{X_A,i\uparrow} \hat{a}_{X_A,i\uparrow} \\
\hat{n}_{iB\downarrow} &= \frac{1}{N_{subl.}} \sum_{X\in B} \hat{a}^{+}_{X_B,i\downarrow} \hat{a}_{X_B,i\downarrow} \\
\Delta n &= \langle \hat{n}_{1A\uparrow} \rangle - \langle \hat{n}_{2A\uparrow} \rangle = \langle \hat{n}_{1B\downarrow} \rangle - \langle \hat{n}_{2B\downarrow} \rangle
\end{aligned}$$

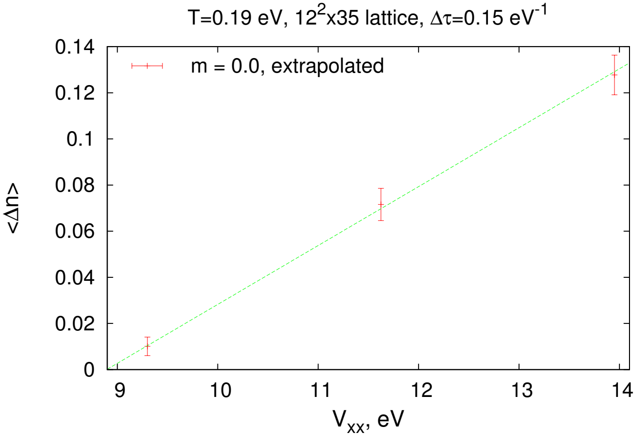
In terms of inverse Dirac operator:

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

AFM condensate and on-site Coulomb interaction



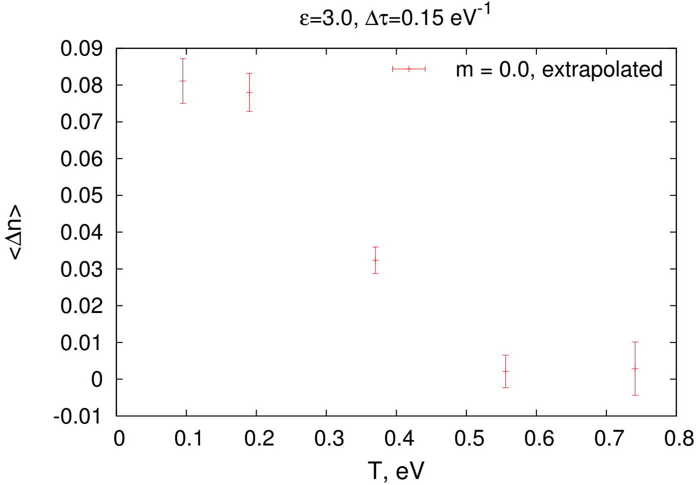
AFM condensate and on-site Coulomb interaction



Our result: $\langle \Delta n \rangle = 0$ nearly at $V_{xx} = 8.9$ eV.
MF result: $\Delta n \approx 0.5$ at $V_{xx} = 8.9$ eV (PRL 109, 206801 (2012)).

AFM condensate and temperature

Taking into account the dielectic substrate: $V_{ij} \to V_{ij}/\epsilon$, except V_{xx}



Conclusions

- Original hexagonal lattice model for AA-bilayer graphene was created
- Long-range Coulomb potentials with screening were taken into account
- Disagreement with the mean-field predictions
- GPUs were used to accelerate calculations
- Computing resources: ITEP Supercomputer, "Lomonosov" Supercomputer at MSU

Work in progress...

Thank you for attention

The end

Fermionic action

$$\begin{aligned} S_\eta &= \sum_{\tau=0}^{N_\tau-1} \sum_{i,j=0}^{1} \sum_{X,Y} \Big[\eta^{*2\tau}_{Xi} \delta_{ij} \delta_{XY} \eta^{2\tau}_{Yj} + \eta^{*2\tau+1}_{Xi} \delta_{ij} \delta_{XY} \eta^{2\tau+1}_{Yj} - \\ &- \eta^{*2\tau}_{Xi} (1 + \Delta\tau A^{ij}_{XY}) \eta^{2\tau+1}_{Yj} - \eta^{*2\tau+1}_{Xi} \delta_{ij} \delta_{XY} \exp^{i\varphi^{2\tau+2}_{Xi}} \eta^{2\tau+2}_{Yj} \Big] = \\ &= \sum_{\tau',\tau=0}^{2N_\tau-1} \sum_{i,j=0}^{1} \sum_{X,Y} \eta^{*\tau'}_{Xi} M^{\tau'\tau}_{XYij} \eta^{\tau}_{Yj}, \end{aligned}$$

where A^{ij}_{XY} is a real matrix and is defined as follows:

$$A^{ij}_{XY} = t\delta_{ij} \left(\delta_{X\in A} \sum_{b=0}^{2} \delta_{Y,X+\rho_b} + \delta_{Y\in B} \sum_{b=0}^{2} \delta_{X,Y-\rho_b} \right) +$$

$$+t_0 \delta_{XY} \left(\delta_{i0}\delta_{j1} + \delta_{i1}\delta_{j0} \right) - m\delta_{ij} \left((-1)^{i+1} \delta_{X_A Y_A} + (-1)^{i} \delta_{X_B Y_B} \right)$$