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 $\sigma$-bonds and the last remains on $\pi$-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?
Monte-Carlo study of the phase transition in the AA-stacked bilayer graphene

Atomic structure and tight-binding Hamiltonian

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

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

\[ a_s = 1.42 \, \text{Å} \]
\[ l_s = 3.3 \, \text{Å} \]
\[ t = 2.57 \, \text{eV} \]
\[ t_0 = 0.36 \, \text{eV} \]
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Tight-binding Hamiltonian

In momentum representation:

\[ \hat{H}_{tb}^k = -\begin{pmatrix} 0 & t_0 & t|f_k| & 0 \\ t_0 & 0 & 0 & t|f_k| \\ t|f_k| & 0 & 0 & t_0 \\ 0 & t|f_k| & t_0 & 0 \end{pmatrix} = -t_0 \hat{\tau}_x \otimes 1 - t_1 \otimes \hat{\sigma}_x |f_k| , \]

where \( f_k = 1 + 2e^{i \frac{3k_x a}{2}} \cos( \frac{k_y a \sqrt{3}}{2} ) \), \( \hat{\tau}_x \) and \( \hat{\sigma}_x \) — Pauli matrices acting in layer space and sublattice space respectively.

Symmetries of the Hamiltonian:

\[ [\hat{\sigma}_x, \hat{H}_{tb}^k] = 0 \Rightarrow \sigma = \pm 1 \quad [\hat{\tau}_x, \hat{H}_{tb}^k] = 0 \Rightarrow \tau = \pm 1 \]
Energy bands without interaction

\[
\begin{align*}
\epsilon_{0k}^{(1)} &= -t_0 - t|f_k|, \quad \sigma = 1, \quad \tau = 1 \\
\epsilon_{0k}^{(2)} &= t_0 - t|f_k|, \quad \sigma = 1, \quad \tau = -1 \\
\epsilon_{0k}^{(3)} &= -t_0 + t|f_k|, \quad \sigma = -1, \quad \tau = 1 \\
\epsilon_{0k}^{(4)} &= t_0 + t|f_k|, \quad \sigma = -1, \quad \tau = -1 \\
\end{align*}
\]

where \( f_k = 1 + 2e^{i\frac{3k_xa}{2}} \cos(\frac{k_ya\sqrt{3}}{2}) \).
E(k) dispersion relation at low energies

\[ \epsilon_F = 0 \Rightarrow \epsilon_{0k}^{(2)} \text{ and } \epsilon_{0k}^{(3)} \text{ form Fermi arcs with the radius } k_r = \frac{2t_0}{3ta}. \]

Near the Dirac points: \[ \epsilon = v_F|k|, \] 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 $\sigma$ and $\tau \Rightarrow$ G-type AFM ordering will break both sublattice and interlayer symmetries and induce energy gap.

Electron densities:

\[
\begin{align*}
n_{1A\uparrow} &= n_{2B\uparrow} = n_{2A\downarrow} = n_{1B\downarrow} = \frac{1 + \Delta n}{2}, \\
n_{1A\downarrow} &= n_{2B\downarrow} = n_{2A\uparrow} = n_{1B\uparrow} = \frac{1 - \Delta n}{2}
\end{align*}
\]

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

AFM condensate: $\Delta n = n_{1A\uparrow} - n_{2A\uparrow} = n_{1B\downarrow} - n_{2B\downarrow}$
G-type AFM ordering may be formed due to the on-site electron-electron interaction$^1$:

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

$^1$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 $\sigma$-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:

$$\hat{q}_{X,i} = \hat{a}^+_{X,i\uparrow}\hat{a}_{X,i\uparrow} + \hat{a}^+_{X,i\downarrow}\hat{a}_{X,i\downarrow} - 1 = \hat{a}^+_{X,i}\hat{a}_{X,i} - \hat{b}^+_{X,i}\hat{b}_{X,i}.$$
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Lattice model

Hamiltonian

Tight-binding Hamiltonian with interaction

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

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

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

\[
\hat{H}_{stag.} = m \sum_{i=1}^{2} \sum_{X, Y} \left[ (-1)^{i+1} \delta_{X_A Y_A} + (-1)^i \delta_{X_B Y_B} \right] (\hat{a}_{X_i}^+ \hat{a}_{Y_i} + \hat{b}_{X_i}^+ \hat{b}_{Y_i})
\]

\[
\hat{H}_{int.} = \frac{1}{2} \sum_{i,j=1}^{2} \sum_{X, Y} \hat{q}_{X_i} V_{XY}^{ij} \hat{q}_{Y_j}, \quad \text{where} \quad \hat{q}_{X_i} = \hat{a}_{X_i}^+ \hat{a}_{X_i} - \hat{b}_{X_i}^+ \hat{b}_{X_i}
\]

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

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

Standard method — inserting Grassmannian coherent states:

\[
|\eta^T \chi^T\rangle = e^{\sum \eta^T_{ Xi} (\hat{a}^+_{ Xi})^T} + e^{\sum \chi^T_{ Xi} (\hat{b}^+_{ Xi})^T} |0\rangle
\]

\[
I = \int D\eta D\eta D\chi D\chi e^{-\sum \chi^T_{ Xi} \chi_{ Xi} - \sum \eta^T_{ Xi} \eta_{ Xi}} \langle \eta^T \chi^T \rangle \langle \eta^T \chi^T | \langle \eta | e^{X,Y} \hat{a}^+_X \hat{a}^-_Y | \eta' \rangle = e^{X,Y} \sum \eta_X (e^A)_{XY} \eta'_Y
\]

Important feature: now we have \(2N_t\) time layers, only even time layers are physical.
It is convenient to perform Hubbard-Stratonovich transformation:

\[ e^{-\frac{\Delta \tau}{2} \sum_{X,Y} \hat{q}_X V_{XY} \hat{q}_Y} = \int D\phi e^{-\frac{1}{2\Delta \tau} \sum_{X,Y} \phi_X V_{XY}^{-1} \phi_Y - i \sum_X \phi_X \hat{q}_X} \]

Finally we arrive at the following expression:

\[ Z = \int D\phi D\tilde{\eta} D\eta D\chi D\bar{\chi} e^{-\tilde{\eta} M \eta - \bar{\chi} M^+ \chi - \frac{1}{2\Delta \tau} \phi^T \hat{V}^{-1} \phi} \]

\[ = \int D\phi \det(M^+ M) e^{-\frac{1}{2\Delta \tau} \phi^T \hat{V}^{-1} \phi} \]

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

**Lattice model**

**AFM condensate**

**Observable: AFM condensate**

**Electron density operators:**

\[
\hat{n}_{iA} = \frac{1}{N_{\text{subl.}}} \sum_{X \in A} \hat{a}_{X,i}^+ \hat{a}_{X,i} \\
\hat{n}_{iB} = \frac{1}{N_{\text{subl.}}} \sum_{X \in B} \hat{a}_{X,i}^+ \hat{a}_{X,i}
\]

\[
\Delta n = \langle \hat{n}_{1A} \rangle - \langle \hat{n}_{2A} \rangle = \langle \hat{n}_{1B} \rangle - \langle \hat{n}_{2B} \rangle
\]

**In terms of inverse Dirac operator:**

\[
\langle \Delta n \rangle = \frac{1}{N_T N_{\text{subl.}}} \sum_{\tau} \left\langle \sum_{X \in A} \left( \hat{M}_{X2X2}^{-1} - \hat{M}_{X1X1}^{-1} \right) \right\rangle \\
= \frac{1}{N_T N_{\text{subl.}}} \sum_{\tau} \left\langle \sum_{X \in B} \left( \hat{M}_{X1X1}^{-1} - \hat{M}_{X2X2}^{-1} \right) \right\rangle
\]
AFM condensate and on-site Coulomb interaction

T = 0.19 eV, $12^2 \times 35$ lattice, $\Delta \tau = 0.15 \text{ eV}^{-1}$

- $V_{xx} = 9.3 \text{ eV}$
- $V_{xx} = 11.625 \text{ eV}$
- $V_{xx} = 13.95 \text{ eV}$
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 dielectric substrate: $V_{ij} \rightarrow V_{ij}/\epsilon$, except $V_{xx}$

$\epsilon=3.0$, $\Delta\tau=0.15$ eV$^{-1}$

$m = 0.0$, extrapolated
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

\[
S_\eta = \sum_{\tau=0}^{N_\tau-1} \sum_{i,j=0}^{1} \sum_{X,Y} \left[ \eta_{X_i}^{*2\tau} \delta_{ij} \delta_{XY} \eta_{Y_j}^{2\tau} + \eta_{X_i}^{*2\tau+1} \delta_{ij} \delta_{XY} \eta_{Y_j}^{2\tau+1} - \eta_{X_i}^{*2\tau} (1 + \Delta \tau A_{XY}^{ij}) \eta_{Y_j}^{2\tau+1} \right. \\
- \left. \eta_{X_i}^{*2\tau+1} \delta_{ij} \delta_{XY} \exp i\varphi_{X_i}^{2\tau+2} \eta_{Y_j}^{2\tau+2} \right] = 2N_\tau - 1 \sum_{\tau',\tau=0}^{1} \sum_{i,j=0}^{X,Y} \eta_{X_i}^{*\tau'} M_{XYij}^{\tau'} \eta_{Y_j}^\tau ,
\]

where \( A_{XY}^{ij} \) is a real matrix and is defined as follows:

\[
A_{XY}^{ij} = t \delta_{ij} \left( \delta_{X \in A} \sum_{b=0}^{2} \delta_{Y,X+\rho_b} + \delta_{Y \in B} \sum_{b=0}^{2} \delta_{X,Y-\rho_b} \right) + \\
+ t_0 \delta_{XY} (\delta_{i0}\delta_{j1} + \delta_{i1}\delta_{j0}) - m \delta_{ij} \left( (-1)^{i+1} \delta_{X_A Y_A} + (-1)^i \delta_{X_B Y_B} \right)
\]