Antiferromagnetic states and phase separation in doped AA-stacked graphene bilayers

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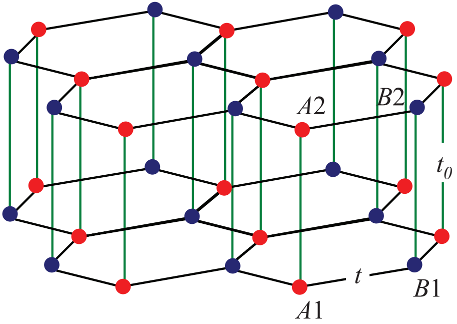
We study electronic properties of AA-stacked graphene bilayers. In the single-particle approximation such a system has one electron band and one hole band crossing the Fermi level. If the bilayer is undoped, the Fermi surfaces of these bands coincide. Such a band structure is unstable with respect to a set of spontaneous symmetry violations. Specifically, strong on-site Coulomb repulsion stabilizes antiferromagnetic order. At small doping and low temperatures, the homogeneous phase is unstable, and experiences phase separation into an undoped antiferromagnetic insulator and a metal. The metallic phase can be either antiferromagnetic (commensurate or incommensurate) or paramagnetic depending on the system parameters. We derive the phase diagram of the system on the doping-temperature plane and find that, under certain conditions, the transition from paramagnetic to antiferromagnetic phase may demonstrate re-entrance. When disorder is present, phase separation could manifest itself as a percolative insulator-metal transition driven by doping.

AA-stacked graphene bilayer



- Not energetically favourable over AB stacking
  $\Rightarrow$ need a pinning mechanism

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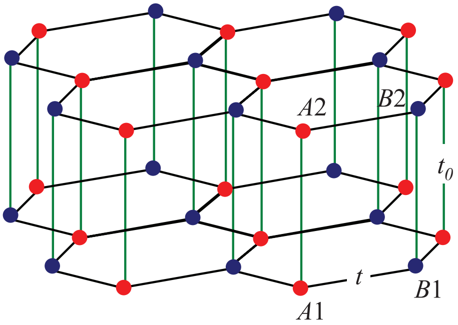

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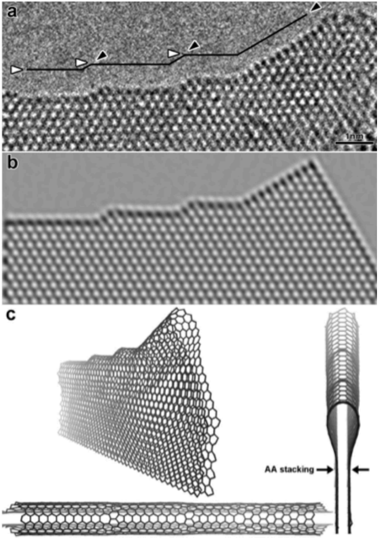
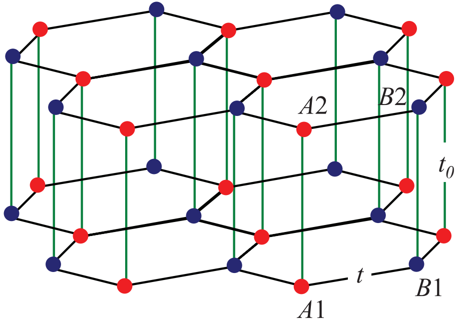


Liu,Suenaga,Harris,Ijima PRL **102**, 015501

Single-particle description



$t \approx 2.57$ eV $\qquad t_0 \approx 0.36$ eV

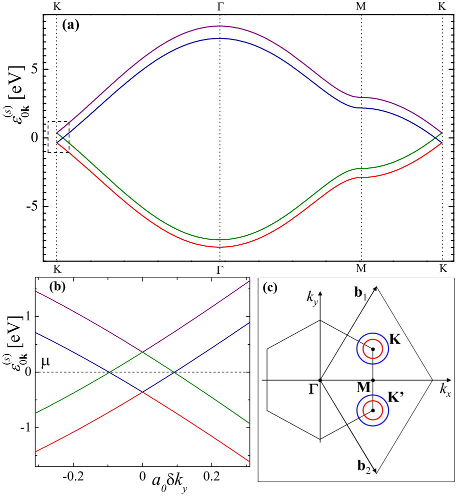
$$
\begin{aligned}
H_0 = & - t \sum_{<\mathbf{nm}>i\sigma} d^\dagger_{\mathbf{n}i\mathcal{A}\sigma} d_{\mathbf{m}i\mathcal{B}\sigma} + \text{H.c.} \\
& - t_0 \sum_{\mathbf{n}a\sigma} d^\dagger_{\mathbf{n}1a\sigma} d_{\mathbf{n}2a\sigma} + \text{H.c.} \\
& - \mu \sum_{\mathbf{n}ia\sigma} d^\dagger_{\mathbf{n}ia\sigma} d_{\mathbf{n}ia\sigma}
\end{aligned}
$$

Spectrum

$$\epsilon^{(1)}_{0\mathbf{k}} = -t_0 - t\zeta_{\mathbf{k}}$$
$$\epsilon^{(2)}_{0\mathbf{k}} = -t_0 + t\zeta_{\mathbf{k}}$$
$$\epsilon^{(3)}_{0\mathbf{k}} = +t_0 - t\zeta_{\mathbf{k}}$$
$$\epsilon^{(4)}_{0\mathbf{k}} = +t_0 + t\zeta_{\mathbf{k}}$$

$$\zeta_{\mathbf{k}} = \left| 1 + 2\exp\left(\frac{3ik_x a_0}{2}\right)\cos\left(\frac{\sqrt{3}k_y a_0}{2}\right)\right|$$

$\Rightarrow$ Twice graphene $\pm t_0$



Fermi surface nesting, prone to instabilities (PRL **109**, 206801 (2012))

Antiferromagnetism with mean field

On-site repulsion $U \sim 4 - 10$ eV

$$H_{\rm int} = \frac{U}{2} \sum_{\mathbf{n}ia\sigma} (n_{\mathbf{n}ia\sigma} - \frac{1}{2})(n_{\mathbf{n}ia\bar{\sigma}} - \frac{1}{2})$$

Order parameter $\Delta_{ia} \equiv U \langle d^{\dagger}_{\mathbf{n}ia\uparrow} d_{\mathbf{n}ia\downarrow} \rangle$ (magnetization along x)

"G-type" $\Delta_{1\mathcal{A}} = \Delta_{2\mathcal{B}} = -\Delta_{1\mathcal{B}} = -\Delta_{2\mathcal{A}} \equiv \Delta$

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$$H^{\rm MF}_{\rm int} = \underbrace{\mathcal{N}\left(\frac{4\Delta^2}{U} - U(n^2 - 1)\right)}_{E_0} + \underbrace{\frac{Ux}{2}\sum_{\mathbf{n}ia\sigma} n_{\mathbf{n}ia\sigma}}_{\mu\to\mu'} - \sum_{\mathbf{n}ia}\Delta_{ia}(d^{\dagger}_{\mathbf{n}ia\uparrow} d_{\mathbf{n}ia\downarrow} + \text{ H.c.})$$

n: #el/site

$x \equiv n - 1$: doping

Self consistency

$$\epsilon_{\mathbf{k}}^{(1,4)} = \mp\sqrt{\Delta^2 + (t\zeta_{\mathbf{k}} + t_0)^2}$$
$$\epsilon_{\mathbf{k}}^{(2,3)} = \mp\sqrt{\Delta^2 + (t\zeta_{\mathbf{k}} - t_0)^2}$$

Minimization of the grand potential w.r.t. Δ

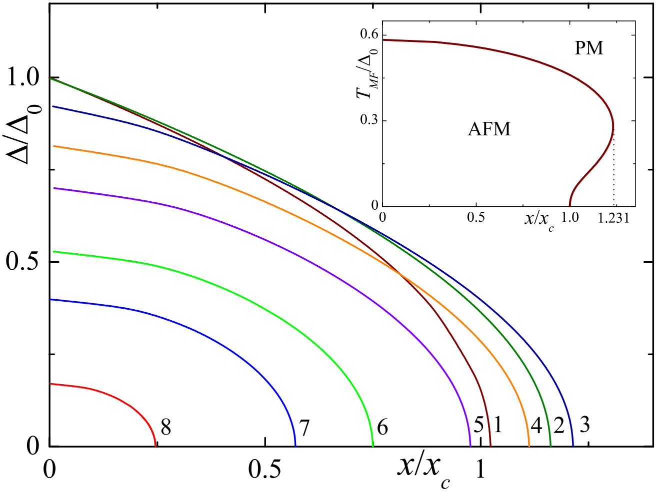
$$\Omega = E_0 - 2T\sum_{s=1}^{4}\int \frac{\mathrm{d}\mathbf{k}}{V_{\mathrm{BZ}}} \log(1 + e^{(\mu' - \epsilon_{\mathbf{k}}^{(s)})/T})$$

Zero temperature

$$\Delta(x,0) = \Delta_0\sqrt{1 - x/x_c}$$
$$\mu'(x,0) = \Delta_0(\mathrm{sgn}(x) - x/2x_c)$$

Transition temperature $T_{\mathrm{MF}} \sim 0.567\Delta_0$ at $x = 0$ for small U

Phase diagram



Re-entrant behavior: ordering with increasing T. Artifact of mean field?

Validity of mean field

- Mermin-Wagner theorem $\Rightarrow$ no magnetic long-range order in 2D

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- Mean field reasonable locally if $\xi_{\mathrm{MF}} < \xi_{\mathrm{sw}}$
- Breakdown of MF $T^* \geq 0.8 T_{\mathrm{MF}}$; T_{MF} still a good estimate of the transition temperature
- MF not quantitatively good for large U

Incommensurate AFM

Spatial modulation of the order parameter $\Delta_{\mathbf{n}ia} \equiv e^{i\mathbf{qn}} U \langle d^\dagger_{\mathbf{n}ia\uparrow} d_{\mathbf{n}ia\downarrow} \rangle$

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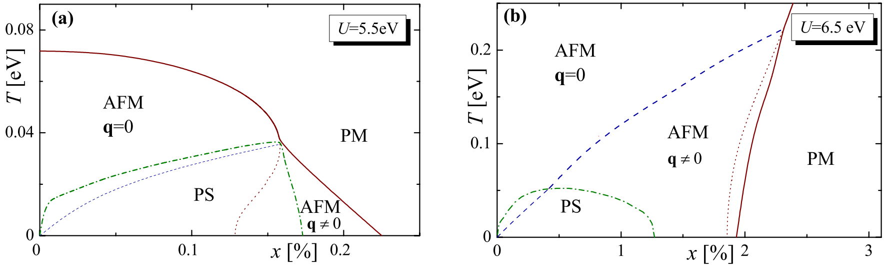
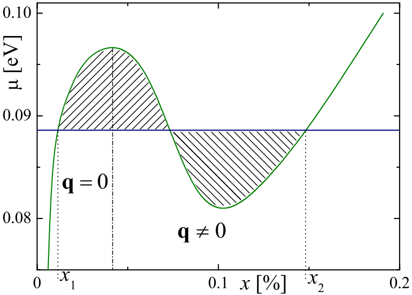


- Incommensurate AFM wins only for low T (less symmetrical)
- Hides re-entrance for low U

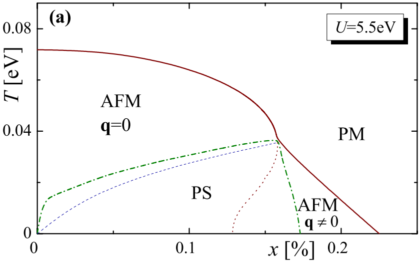
Phase separation

In some regions of (x, T), $\partial\mu/\partial x < 0 \Rightarrow$ unphysical
Separation of two phases (comm. AFM, incomm. AFM) with locked electron densities x_1, x_2

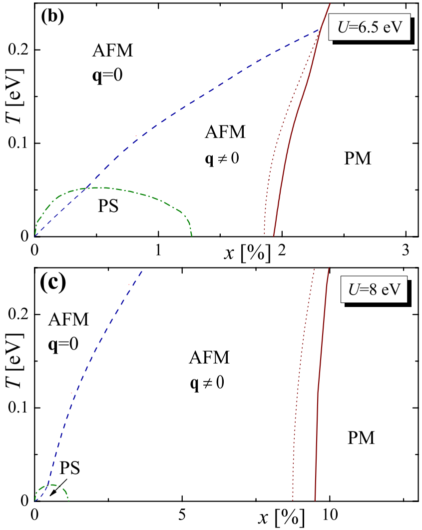


$x2 \gg x1 \Rightarrow$ percolative metal-‘insulator’ transition upon doping (arXiv:1302.1994)

Phase diagram

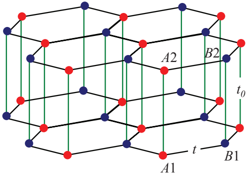


- Actual values of x_c, T_c strongly depend on U
  $T_c \sim 50$ K for $U = 5.5$ eV
  $T_c \geq$ RT for $U \geq 6.5$ eV



Conclusions

- Magnetic properties of AA-stacked bilayer graphene



- Antiferromagnetism observable (maybe up to RT)
- Possibility of re-entrance, incommensurate AFM, phase separation and percolative metal-insulator transition; some may be artifacts

Series of papers by the same authors: PRL **109**, 206801; PRB **87**, 075128; PRB **87**, 121401; arXiv 1302.1994; arXiv 1305.0330