Known and unknown about graphene.

I. Graphene 101: pure and disordered monolayer graphene.

Lectures 3&4 II. Electronic properties of bilayer graphene, from high to low energies. Interaction effects in graphenes.

Electron-electron interaction in monolayers.

Tight-binding model for electrons in BLG.

Asymmetry gap in bilayer graphene.

Lifshitz transitions & BLG under strain.



Interaction effects in BLG; spontaneous symmetry breaking in pristine BLG due to the e-e interaction.

Wallace, Phys. Rev. 71, 622 (1947) Slonczewski, Weiss, Phys. Rev. 109, 272 (1958)



Eigenfunction

$$\Psi_{j}(\mathbf{k},\mathbf{r}) = \sum_{i=1}^{2} C_{ji}(\mathbf{k}) \Phi_{i}(\mathbf{k},\mathbf{r})$$

Transfer integral on a hexagonal lattice

$$\mathcal{H}_{AB} = \langle \Phi_A | H | \Phi_B \rangle$$

Brillouin zone ky (valleys) K' V kx

 $\pi = p_x + ip_y = pe^{i\vartheta}$

$$\mathcal{H}_{AB} = \underbrace{1}_{N} \sum_{\mathbf{R}_{A}, \mathbf{R}_{B}}^{N} e^{i\mathbf{k}(\mathbf{R}_{B} - \mathbf{R}_{A})} \underbrace{\langle \phi_{A}(\mathbf{r} - \mathbf{R}_{A}) | \mathbf{H} | \phi_{B}(\mathbf{r} - \mathbf{R}_{B})}_{\gamma_{0} \sim 3eV} = \gamma_{0} \begin{bmatrix} e^{-i\frac{2\pi}{3}} e^{-i(\frac{a}{2}p_{x} + \frac{a}{2\sqrt{3}}p_{y})} + e^{i\frac{a}{\sqrt{3}}p_{y}} + e^{i\frac{2\pi}{3}} e^{i(\frac{a}{2}p_{x} - \frac{a}{2\sqrt{3}}p_{y})} \end{bmatrix}$$

$$\approx \frac{\sqrt{3}}{2} \gamma_{0} a(p_{x} - ip_{y}) = v\pi^{+}$$

$$H_{BA,K} \approx \frac{\sqrt{3}}{2} \gamma_{0} a(p_{x} + ip_{y}) = v\pi$$

$$\hat{H} = v \begin{pmatrix} 0 & \pi^{+} \\ \pi & 0 \end{pmatrix} = v\vec{p} \cdot \vec{\sigma}$$

McClure, PR 104, 666 (1956)





Also, one may need to take into account an additional real spin degeneracy of all states

$$H = \int d\vec{r} \ \psi_r^+ v \vec{\sigma} \cdot (-i\nabla) \psi_r + \frac{1}{2} \int d\vec{r} d\vec{r}' \ \frac{e^2}{|\vec{r} - \vec{r}'|} \psi_r^+ \psi_r \psi_r^+ \psi_{r'} \psi_{r'}^+ \psi_{r'} \psi_{r'}^+ \psi_{r'} \psi_{$$

$$v(\varepsilon) \rightarrow v + \frac{e^2}{8\chi v} \ln \frac{\gamma_0}{\varepsilon}$$
Gonzalez, Guinea, Vozmediano - PRB 59, 2474 (1999)
$$-\frac{2\pi e^2}{q}$$
unscreened, if
$$\frac{e^2}{\chi v} < 1$$
dynamically screened
$$-\tilde{v}(q,\omega) = \frac{-2\pi e^2/q}{1+N\Pi 2\pi e^2/q} \rightarrow \frac{-1}{N\Pi(q,\omega)}$$
if
$$\frac{e^2}{\chi v} > 1$$

$$\frac{dv}{d\ln \frac{\gamma_0}{\varepsilon}} = \frac{4}{\pi^2 N} v \implies \varepsilon(p) = Cp^{1-\delta - 0.9 \div 1}$$
Son - PRB 75, 235423 (2007)

 g_l^n remain small (do not renormalize up)

Aleiner, Kharzeev, Tsvelik – PRB 76, 195415 (2007) Drut, Son – PRB 77, 075115 (2008)

Renormalisation of Dirac velocity in suspended monolayer graphene



Elias, Gorbachev, Mayorov, Morozov, Zhukov, Blake, Ponomarenko, Grigorieva, Novoselov, Guinea, Geim Nature Physics 7, 701 (2011)

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Minimal TB model for electrons in BLG





$$\begin{array}{c|c} D_{3d} + T_a D_{3d} + T_a^2 D_{3d} \\ \\ \text{IrReps} \\ \end{array}$$

$$\begin{array}{c|c} sublattice valley \\ \hline \sigma_n \begin{pmatrix} \varphi_{A,+} \\ \varphi_{\tilde{B}+} \\ -\varphi_{A-} \end{pmatrix} \\ \hline \tau_l \\ \hline \sigma_n \begin{pmatrix} \varphi_{A,-} \\ \varphi_{\tilde{B}-} \\ -\varphi_{A-} \end{pmatrix} \\ \hline \tau_l \\ \hline \sigma_n \begin{pmatrix} \varphi_{A,-} \\ \varphi_{\tilde{B}-} \\ -\varphi_{A-} \end{pmatrix} \\ \hline \tau_l \\ \hline \sigma_n - \tau_l \\ \hline \sigma_n \rightarrow - \sigma_n \\ \hline \tau_l \rightarrow - \tau_l \\ \hline \sigma_n \tau_l \rightarrow \sigma_n \tau_l \\ \hline \end{array}$$

$$\begin{array}{c|c} t \rightarrow -t \\ \sigma_n \tau_l \rightarrow -\sigma_n \\ \hline \tau_l \rightarrow -\sigma_n \\ \hline \sigma_n \tau_l \rightarrow \sigma_n \tau_l \\ \hline \end{array}$$

$$\begin{array}{c|c} t \rightarrow -t \\ \sigma_n \tau_l \rightarrow \sigma_n \tau_l \\ \hline \sigma_n \tau_l \rightarrow \sigma_n \tau_l \\ \hline \end{array}$$

$$\begin{array}{c|c} t \rightarrow -t \\ \sigma_n \tau_l \rightarrow -\sigma_n \\ \hline \sigma_n \tau_l \rightarrow \sigma_n \tau_l \\ \hline \end{array}$$

$$\begin{array}{c|c} t \rightarrow -t \\ \sigma_n \tau_l \rightarrow \sigma_n \tau_l \\ \hline \end{array}$$

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$$\begin{array}{c|c} t \rightarrow -t \\ \sigma_n \tau_l \rightarrow \sigma_n \tau_l \\ \hline \end{array}$$



$$H_{BLG} = \frac{\tau_{z}}{2m} \vec{\sigma} \cdot (p_{y}^{2} - p_{x}^{2}, 2p_{x}p_{y})$$

$$H = v\xi\begin{pmatrix} 0 & \pi^{+} \\ \pi & 0 \end{pmatrix}$$
energy scale $\hbar v/\lambda_{B}$
where $\lambda_{B} = \sqrt{\frac{\hbar}{eB}}$
state at zero energy:
 $\pi \phi_{0} = 0$

$$H = -\frac{1}{2m}\begin{pmatrix} 0 & (\pi^{+})^{2} \\ \pi^{2} & 0 \\ 0 \end{pmatrix}$$
energy scale $\hbar w_{c}$
where $\omega_{c} = \frac{eB}{m}$
 $m \approx 0.035m_{c}$

$$\frac{f^{2} + (1, +)(1, -)}{\pi^{2} \phi_{0} = 0}$$

$$\frac{e^{f\hbar\omega_{c}} \uparrow \downarrow}{\sqrt{2} + (1, +)(1, -)}$$

$$\frac{e^{f\hbar\omega_{c}} \uparrow \downarrow}{\sqrt{2} + (1, +)(1, -)}$$

$$\frac{e^{f\hbar\omega_{c}} \uparrow \downarrow}{\sqrt{2} + (1, +)(1, -)}$$

$$\frac{e^{f}\omega_{c}}{\sqrt{2} + (2, +)(2, -)}$$

$$\frac{e^{f}\omega_{c$$

086805 (2006)



Quantum Hall effect in bilayer graphene



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Tight-binding model for electrons in BLG.

Lifshitz transitions & BLG under strain.

Asymmetry gap in bilayer graphene.



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$$\hat{H} = \frac{1}{2m} \tau_{3} \vec{\sigma} \cdot (p_{y}^{2} - p_{x}^{2}, 2p_{x}p_{y}) + v_{3} \vec{\sigma} \cdot \vec{p}$$

$$= -\frac{\tau_{3}}{2m} \begin{pmatrix} 0 & \pi^{2} \\ (\pi^{+})^{2} & 0 \end{pmatrix} + v_{3} \begin{pmatrix} 0 & \pi^{+} \\ \pi & 0 \end{pmatrix}$$

$$E_{LITr} = \frac{m_{3}^{2}}{2} \sim ImeV$$

$$h_{LITr} = \frac{2}{\pi^{2}} \left(\frac{mv_{3}}{\hbar}\right)^{2} \sim 10^{10} cm^{-2}$$

-

strained monolayer graphene





$$\gamma_0 e^{-i\frac{2\pi}{3}} + \gamma_0 + \gamma_0 e^{i\frac{2\pi}{3}} = 0$$



$$\hat{H} = v\vec{p}\cdot\vec{\sigma} + \zeta\vec{u}\cdot\vec{\sigma} \equiv v[\vec{p} + \frac{\tau_3}{v}\vec{u}]\cdot\vec{\sigma}$$

shift of the Dirac point in the momentum space, opposite in K/K' valleys, like vector potential

$$B_{eff} = \tau_3 [\nabla \times \vec{u}(\vec{r})]_z$$

lordanskii, Koshelev, JETP Lett 41, 574 (1985) Ando - J. Phys. Soc. Jpn. 75, 124701 (2006)

Iordanskii, Koshelev, JETP Lett 41, 574 (1985) Morpurgo, Guinea - PRL 97, 196804 (2006) The four-band Hamiltonian for one DP in BLG:

$$\hat{H} = \begin{pmatrix} 0 & \xi v_3 \hat{\pi} + \mathcal{A}_3 & 0 & \xi v \hat{\pi}^\dagger + \mathcal{A}_0^* \\ \xi v_3 \hat{\pi}^\dagger + \mathcal{A}_3^* & 0 & \xi v \hat{\pi} + \mathcal{A}_0 & 0 \\ 0 & \xi v \hat{\pi}^\dagger + \mathcal{A}_0^* & 0 & \gamma_1 \\ \xi v \hat{\pi} + \mathcal{A}_0 & 0 & \gamma_1 & 0 \end{pmatrix}$$
$$\psi \rightarrow \psi \exp \left\{ -\frac{i\xi}{\hbar v} (x \Re \mathcal{A}_0 + y \Im \mathcal{A}_0) \right\} \qquad \text{Vector potential}$$

Removes constant vector potential from the anti-diagonal

$$H = \begin{pmatrix} 0 & v_3 \pi + w & 0 & v \pi^{\dagger} \\ v_3 \pi^{\dagger} + w^* & 0 & v \pi & 0 \\ 0 & v \pi^{\dagger} & 0 & \gamma_1 \\ v \pi & 0 & \gamma_1 & 0 \end{pmatrix}$$

$$w = \frac{3}{4}(\delta - \delta')\gamma_3(\eta_3 - \eta_0)e^{-i2\theta} - \frac{3}{2}\gamma_3\eta_3\frac{\delta r}{r_{AB}}e^{i\varphi}$$

high-energy
4-band:

$$H = \begin{pmatrix} 0 & v_3 \pi + w & 0 & v \pi^{\dagger} \\ v_3 \pi^{\dagger} + w^* & 0 & v \pi & 0 \\ 0 & v \pi^{\dagger} & 0 & \gamma_1 \\ v \pi & 0 & \gamma_1 & 0 \end{pmatrix}$$
Iow-energy
2-band:

$$H = -\frac{1}{2m} \begin{pmatrix} 0 & (\pi^{\dagger})^2 \\ \pi^2 & 0 \end{pmatrix} + v_3 \begin{pmatrix} 0 & \pi \\ \pi^{\dagger} & 0 \end{pmatrix} + \begin{pmatrix} 0 & w \\ w^* & 0 \end{pmatrix}$$

$$w = \frac{3}{4} (\delta - \delta') \gamma_3 (\eta_3 - \eta_0) e^{-i2\theta} - \frac{3}{2} \gamma_3 \eta_3 \frac{\delta r}{r_{AB}} e^{i\varphi}$$

Mucha-Kruczynski, Aleiner, VF - PRB 84, 041404 (2011)

$$\eta_{0} = \frac{d \ln \gamma_{0}}{d \ln r_{AB}} \approx -3 \quad \text{(Raman and DFT) Basko et al., PRB 80, 165413 (2009)} \quad \eta_{3} = \frac{d \ln \gamma_{3}}{d \ln r_{AB}} << \frac{d \ln \gamma_{0}}{d \ln r_{AB}}$$

Strain effect on the BLG spectrum at low energies





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eV

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Interlayer asymmetry gap in bilayer graphene

$$\hat{H}_{2} = -\frac{v^{2}}{\gamma_{1}} \begin{pmatrix} 0 & (\pi^{\dagger})^{2} \\ \pi^{2} & 0 \end{pmatrix} + \begin{pmatrix} u & 0 \\ 0 & -u \end{pmatrix}$$
(can be controlled using electrostatic gates)



McCann & VF - PRL 96, 086805 (2006) McCann - PRB 74, 161403 (2006) Castro, et al - PRL 99, 216802 (2007)



T. Ohta et al - Science 313, 951 (2006)







Zhang, et al - Nature 459, 820 (2009)

Gate defined quantum confinement in suspended bilayer graphene



С

nergy

Allen, Martin, Yacoby - arXiv:1202.0820

Interlayer asymmetry-gap can be used to induce confinement in BLG to make quantum dots for spin qubits.

VF – Nature Physics 3, 151 (2007)

Encapsulation of BLG in BN films improves performance QDs circuits (larger gaps better controlled by the gates).

Vandersypen's group, Delft (2012)

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Screening of Coulomb interaction in BLG



Asymmetry gap in bilayer graphene: a strongly correlated band insulator.

Spontaneous symmetry breaking in pristine BLG due to the e-e interaction.



2D-screened Coulomb interaction:

$$V(q) = \frac{2\pi e^2}{q} \implies \tilde{V}(q < a_{scr}^{-1}, \omega = 0) \rightarrow \frac{2\pi e^2}{q + Na_{Bohr}^{-1}} \xrightarrow{q \to 0} \frac{1}{Nm}$$

$$(arge' N = 4 \implies 1/N \text{ expansion}$$

$$justifying the use of perturbation theory$$

$$a_{Bohr} \sim 30\dot{A} \qquad r$$

produces a negligibly small renormalisation of the band mass

$$\frac{d \ln m}{d \ln p} \sim 10^{-2}$$
 Lemonik, Aleiner, Toke, VF PRB 82, 201408 (2010)

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$$\varepsilon_{e/h} = \sqrt{\left(\frac{p^2}{2m}\right)^2 + u^2} \approx u + \frac{p^4}{8m^2u}$$



imperfect 2D screening





single electron/hole

el-hole excitations



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Asymmetry gap in bilayer graphene (strongly correlated band insulator).



Spontaneous symmetry breaking in pristine BLG due to the e-e interaction.

Is 'vacuum state' in pristine bilayer graphene stable against spontaneous symmetry breaking due to e-e interaction?

for BLG in a zero magnetic field, there were several suggestions:

ferroelectric 'excitonic insulator'

Nandkishore, L. Levitov, -PRL104, 156803 (2010); Jung, Zhang, MacDonald - PRB 83, 115408 (2011)

layer polarized antiferromagnetic

Kharitonov arXiv:1109.1553; Min, Borghi, Polini, MacDonald - PRB 77, 041407(2008); Vafek - PRB 82 205106 (2010)

quantum anomalous Hall state

Nandkishore, Levitov - PRB 82, 115124 (2010); Zhang, Jung, Fiete, Niu, MacDonald - PRL106, 156801 (2011)

charge density wave state

Dahal, Wehling, Bedell, Zhu, Balatsky - Physica B 405, 2241 (2010)

nematic (breaking rotational symmetry)

Vafek, Yang - PRB 81, 041401 (2010), Lemonik, Aleiner, Toke, VF - PRB 82, 201408 (2010)

nematic, antiferromagnetic, spin flux state.

Lemonik, Aleiner, VF - PRB 85, 245451 (2012)

interaction-driven phases of electronic liquid in bilayer graphene

$$H_{s-p} = -\frac{1}{2m} \left[(p_x^2 - p_y^2) \sigma_1 - 2 p_x p_y \sigma_2 \right] \tau_3 + v_3 \vec{p} \cdot \vec{\sigma}$$

Irreps. R

strain $g_3^1 = g_3^2 = g_{E_2}$ interlayer asymmetry $g_3^3 = g_{B_2}$ $g_0^3 = g_{A_2}$ $g_3^0 = g_{B_1}$ $g_1^3 = g_2^3 = g_{F''}$ charge-density wave $g_1^0 = g_2^0 = g_{F'}$ $g_0^1 = g_0^2 = g_{E_1}$ $g_1^1 = g_2^2 = g_1^2 = g_2^1 = g_G$

 $H_{C} = \frac{e^{2}}{2} \int d^{2}r d^{2}r' \frac{\psi_{r}^{+}\psi_{r} \psi_{r'}^{+}\psi_{r'}}{|r-r'|}$

$$H_{sr} = \frac{2\pi}{m} \sum_{l,n=0123} g_l^n \int d^2 r \left[\psi_r^+ \sigma_n \tau_l \psi_r \right]^2$$

sublattice valley

electron spin degree of freedom included and used when calculating exchange energy



construction blocks

one interaction, mean field theory & Hartree-Fock

$$H_{sr} = -\frac{2\pi}{m} |g| \int d^{2}r \left[\psi_{r}^{+}\hat{R}\psi_{r}\right]^{2} \Delta = |g| \left\langle\psi_{r}^{+}\hat{R}\psi_{r}\right\rangle$$
$$E_{MF} = -N \int_{\frac{k^{2}}{2m} < \frac{\gamma_{1}}{2}} \frac{kdk}{2\pi} \varepsilon(k, \Delta) + \frac{m\Delta^{2}}{8\pi c_{R} |g|}$$
$$= const - N \frac{m\Delta^{2}}{8\pi} \left(\alpha + \beta \ln \frac{\gamma_{1}}{\Delta}\right) + \frac{m\Delta^{2}}{8\pi b_{R} |g|} = \min$$

$$T_c \sim \Delta \sim \gamma_1 e^{-\frac{\#}{N|g|}}$$

The expected small bare values of *g* determines an exponentially weak phase transition (BCS)

construction blocks

renormalisation of one interaction followed by mean field theory & Hartree-Fock

$$\int \int \int e^{-\frac{\pi}{2}} e^{-\frac{\pi}{N|g(\gamma_{1})|}} \frac{d\omega d^{2}q}{(\omega - q^{2})^{2}} \sim -Ng^{2} \ln \frac{\gamma_{1}}{\varepsilon}$$

$$g(\gamma_{1}) <<1$$

$$\frac{dg}{dl} = -\#Ng^{2} \Rightarrow g(\varepsilon) = \frac{g(\gamma_{1})}{1 + \#Ng(\gamma_{1})\ln(\gamma_{1}/\varepsilon)}$$

$$g(\varepsilon_{c}) \rightarrow \infty$$

$$\int \frac{T_{c} \sim \varepsilon_{c} \sim \gamma_{1}e^{-\frac{\#}{N|g(\gamma_{1})|}}}{for one attractive interaction gives the same as MF-FH.}$$

$$L$$

$$g(\varepsilon_{c}) \sim 1$$



For one interaction channel, E₂ renormalisation of g can be helped by Coulomb interaction even more:



 $\frac{dg_{E_2}}{dl} = \dots$ # $\overline{N^2}$



L

<u>Altogether</u>: simultaneous renormalisation group analysis of <u>all</u> short-range interactions helped by screened Coulomb interaction



Renormalisation of short-range interactions



$$\begin{split} \delta(E_2)_{i=3}^{j=1,2} &= 1 \text{ and } \delta(E_2)_i^j = 0 \text{ otherwise} \\ \downarrow \\ \frac{dg_i^j}{d\ell} &= -\frac{\tilde{\alpha}\delta(E_2)_i^j}{N^2} - \frac{\alpha_1 g_i^j}{N} - \frac{NB_i^j \left(g_i^j\right)^2 - \sum_{k,l,m,n=0}^3 C_{i;km}^{j;ln} \tilde{g}_k^l \tilde{g}_m^n \end{split}$$



 $\delta H \propto \left\langle \psi \psi^{+} \right\rangle$

Nematic $\sigma_{1,2}\tau_3$ mimics effect of strain: gaplesss with LiTr

AntiFerro $\sigma_3 \tau_3 \vec{s} \vec{l}$ opposite spin polarisation on A and B sublattices in the opposite layers: gapped

*SpinFlux σ*3*sl* like SO – topological insulator, 'spin Hall'



Density of thermally activated carriers (electrons and holes) in suspended neutral BLG



Mayorov, Elias, Mucha-Kruczynski, Gorbachev, Tudorovskiy, Zhukov, Morozov, Katsnelson, VF, Geim Science 333, 860 (2011)



Gapless persistence of **v=4** SdHO to the lowest fields with activation energy indicating LiTr, **Nematic** (or strain ?)

Suppressed compressibility and conductance Persistence of *v=4* SdHO to the lowest fields: what is the phase?

Feldman, Martin, Yacoby, Nature Physics 5, 889 (2009)

(10°/cm²)

=

0

0.2

0.4

Weitz, Allen, Feldman, Martin, Yacoby Science 330, 812 (2010)

Bao, Velasco, Zhang, Jing, Standley, Smirnov, Bockrath, MacDonald, Lau arXiv:1202.3212



(10ⁿ/cm²)

0.2

0.4

Gapped state AntiFerro ?

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