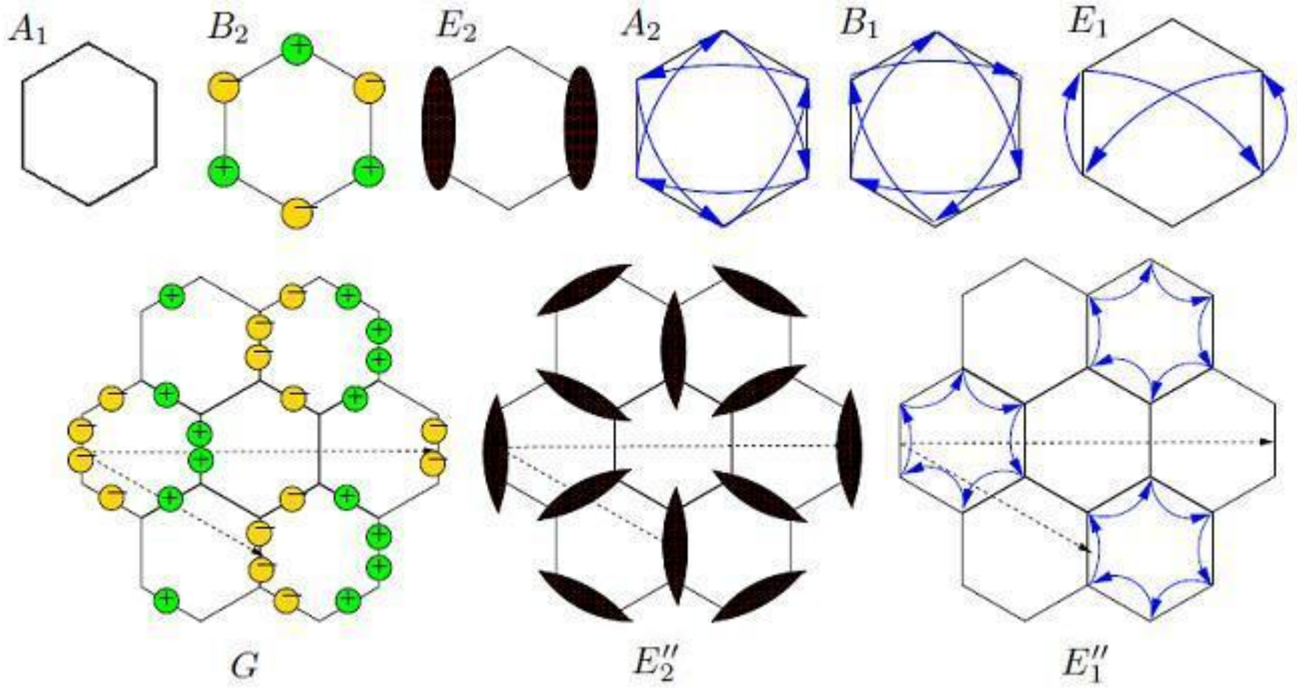
A Renormalization Group Study of the Ground State of Bilayer Graphene

Y. Lemonik (Columbia U, New York, USA)

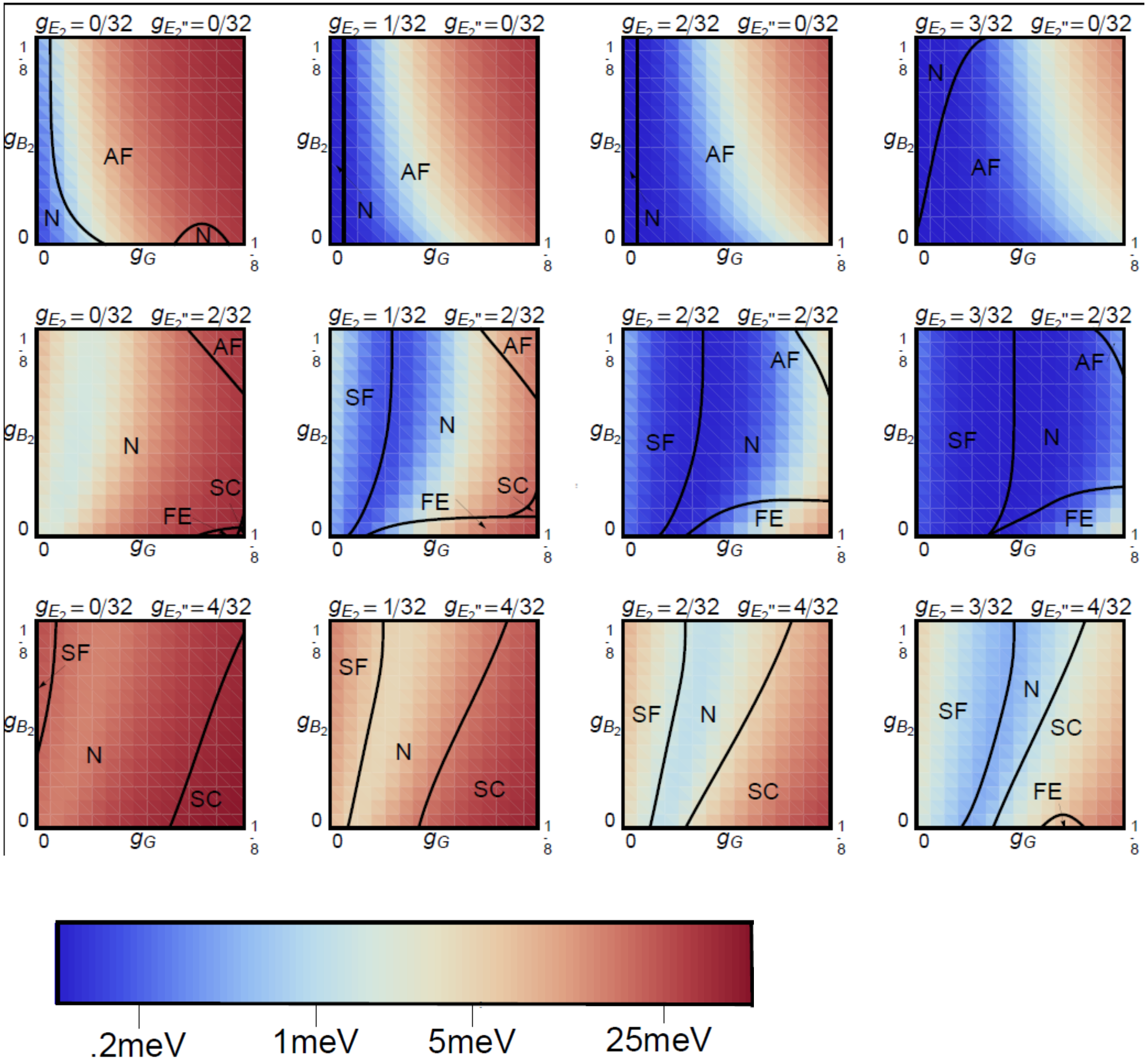
Y. L., I.Aleiner, C. Toke, & V.I. Falko, PRB 82, 201408(R) (2010)
Y. L., I.Aleiner, & V.I. Falko *(in preparation)*

I. Bilayer Graphene
II. Hamiltonian & Interactions
III. Renormalization Group Flow of Interaction Constants
IV. Termination of RG & Mean Field Analysis
V. Phases



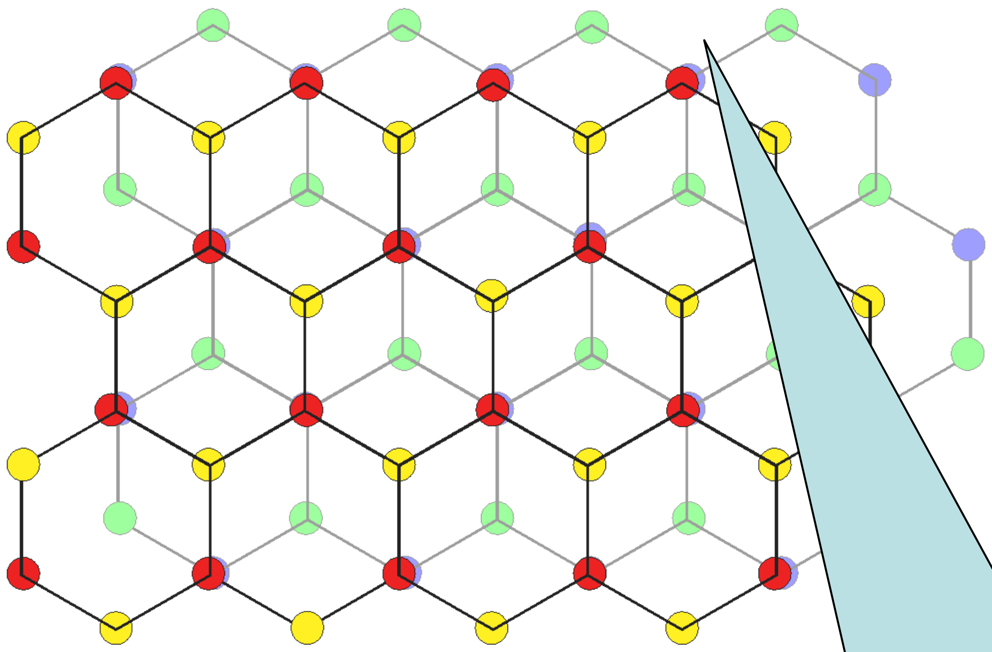
Warning: presented results are obtained using 1/N expansion, N=4.

Results:



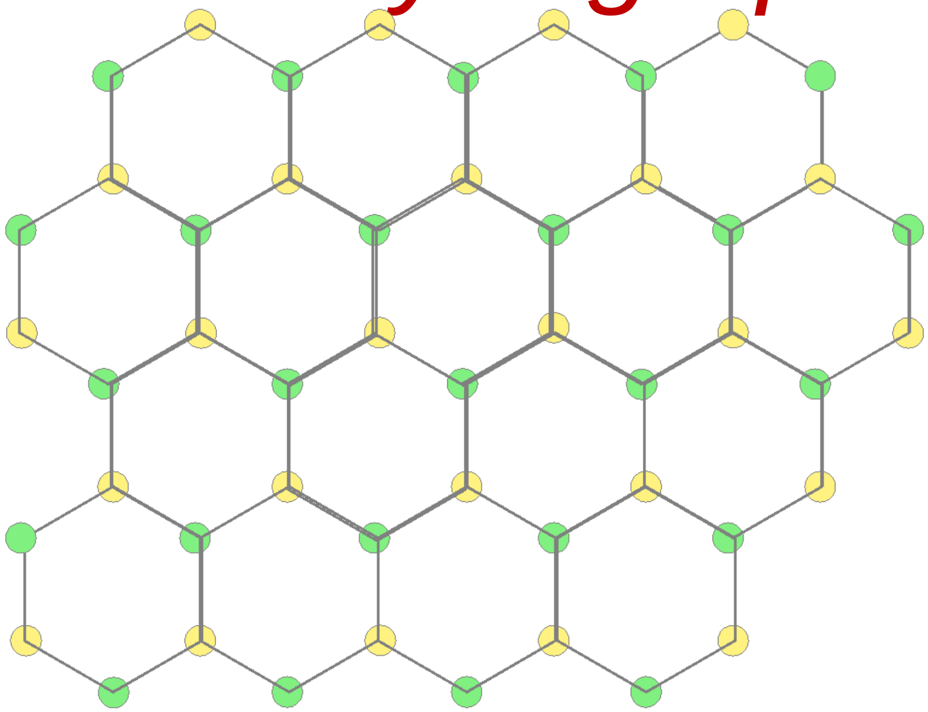
AF – Antiferromagnetic
N – Nematic
SF – Spin Flux
FE – Ferroelectric (unlikely)
SC – Triplet Superconductor

Bilayer graphene (intro)



Dimers hybridization energy 0.4 eV; split bands can be removed from the four band model.

Bilayer graphene (intro)



$$\vec{u} \equiv \begin{pmatrix} u_K^A \\ u_K^B \\ u_{K'}^B \\ -u_{K'}^A \end{pmatrix}$$

Only low energy sites are left: two band model on the honeycomb lattice.

$$\hat{H}_0 = \frac{1}{2m} \int d^2\mathbf{r} \psi^\dagger \left\{ \hat{\tau}_3^{KK'} \otimes \left[\left(\partial_y^2 - \partial_x^2 \right) \hat{\tau}_1^{AB} - 2\partial_x \partial_y \hat{\tau}_2^{AB} \right] \right\} \psi$$

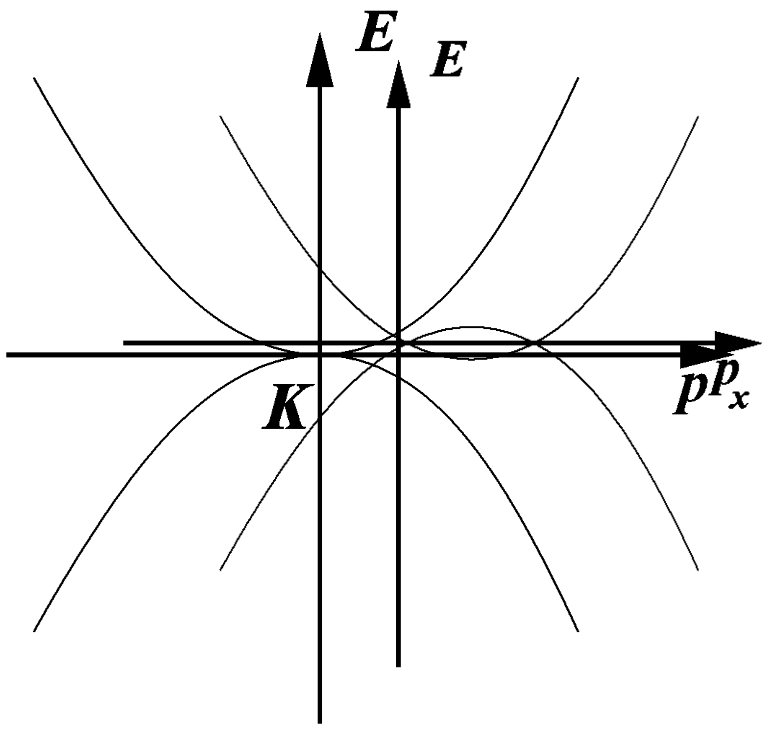
Hopping via dimer

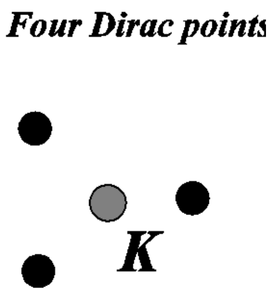
$$+ v_3 \int d^2\mathbf{r} \psi^\dagger \left\{ \mathbb{1}^{KK'} \otimes \left[-i\partial_x \hat{\tau}_1^{AB} - i\partial_y \hat{\tau}_2^{AB} \right] \right\} \psi$$

Small direct tunneling

Spectrum of non-interacting electrons:

$$\hat{H}_0 = \gamma \int d^2\mathbf{r}\psi^\dagger \left\{ \hat{\tau}_3^{KK'} \otimes \left[\left(\partial_y^2 - \partial_x^2 \right) \hat{\tau}_1^{AB} - 2\partial_x \partial_y \hat{\tau}_2^{AB} \right] \right\} \psi$$





In a wide energy interval the spectrum is parabolic

Interaction Hamiltonian

$$\hat{H}_0 = \frac{1}{2m}\int d^2\mathbf{r}\psi^\dagger \left\{\hat{\tau}_3^{KK'} \otimes \left[\left(\partial_y^2 - \partial_x^2\right)\hat{\tau}_1^{AB} - 2\partial_x\partial_y\hat{\tau}_2^{AB}\right]\right\}\psi$$

$$- iv_3 \int d^2\mathbf{r}\psi^\dagger \left\{\partial_x\hat{\tau}_1^{AB} + \partial_y\hat{\tau}_2^{AB}\right\}\psi$$

Relevant

$$+ \frac{e^2}{2}\int d\mathbf{r}d\mathbf{r}' \frac{\left[\psi^\dagger\psi\right](\mathbf{r})\left[\psi^\dagger\psi\right](\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

$$+ \frac{2\pi}{m}\sum_{i,j=0}^{3} g_j^i \int d\mathbf{r}\left[\psi^\dagger\hat{\tau}_i^{AB}\otimes\hat{\tau}_j^{KK'}\psi\right]^2$$

marginal

Symmetries:

$$g_{xx} = g_{xy} = g_{yx} = g_{yy} \equiv g_G$$

$$g_{xz} = g_{yz} \equiv g_{E_2};\ g_{zx} = g_{zy} \equiv g_{E_2''}$$

$$g_{x0} = g_{y0} \equiv g_{E_1};\ g_{0x} = g_{0y} \equiv g_{E_1''}$$

$$g_{z0} \equiv g_{B_1};\ g_{0z} \equiv g_{A_2};\ g_{zz} \equiv g_{B_2}$$

9 couplings

Current-Current & Density-Density

Interaction Hamiltonian

$$\hat{H}_0 = \frac{1}{2m}\int d^2\mathbf{r}\psi^\dagger \left\{\hat{\tau}_3^{KK'}\otimes\left[\left(\partial_y^2-\partial_x^2\right)\hat{\tau}_1^{AB}-2\partial_x\partial_y\hat{\tau}_2^{AB}\right]\right\}\psi$$

$$-iv_3\int d^2\mathbf{r}\psi^\dagger\left\{\partial_x\hat{\tau}_1^{AB}+\partial_y\hat{\tau}_2^{AB}\right\}\psi$$

$$+\frac{e^2}{2}\int d\mathbf{r}d\mathbf{r}'\,\frac{\left[\psi^\dagger\psi\right](\mathbf{r})\left[\psi^\dagger\psi\right](\mathbf{r}')}{\left|\mathbf{r}-\mathbf{r}'\right|}$$

Relevant

$$+\frac{2\pi}{m}\sum_{i,j=0}^{3} g_j^i\int d\mathbf{r}\left[\psi^\dagger\hat{\tau}_i^{AB}\otimes\hat{\tau}_j^{KK'}\psi\right]^2$$

marginal

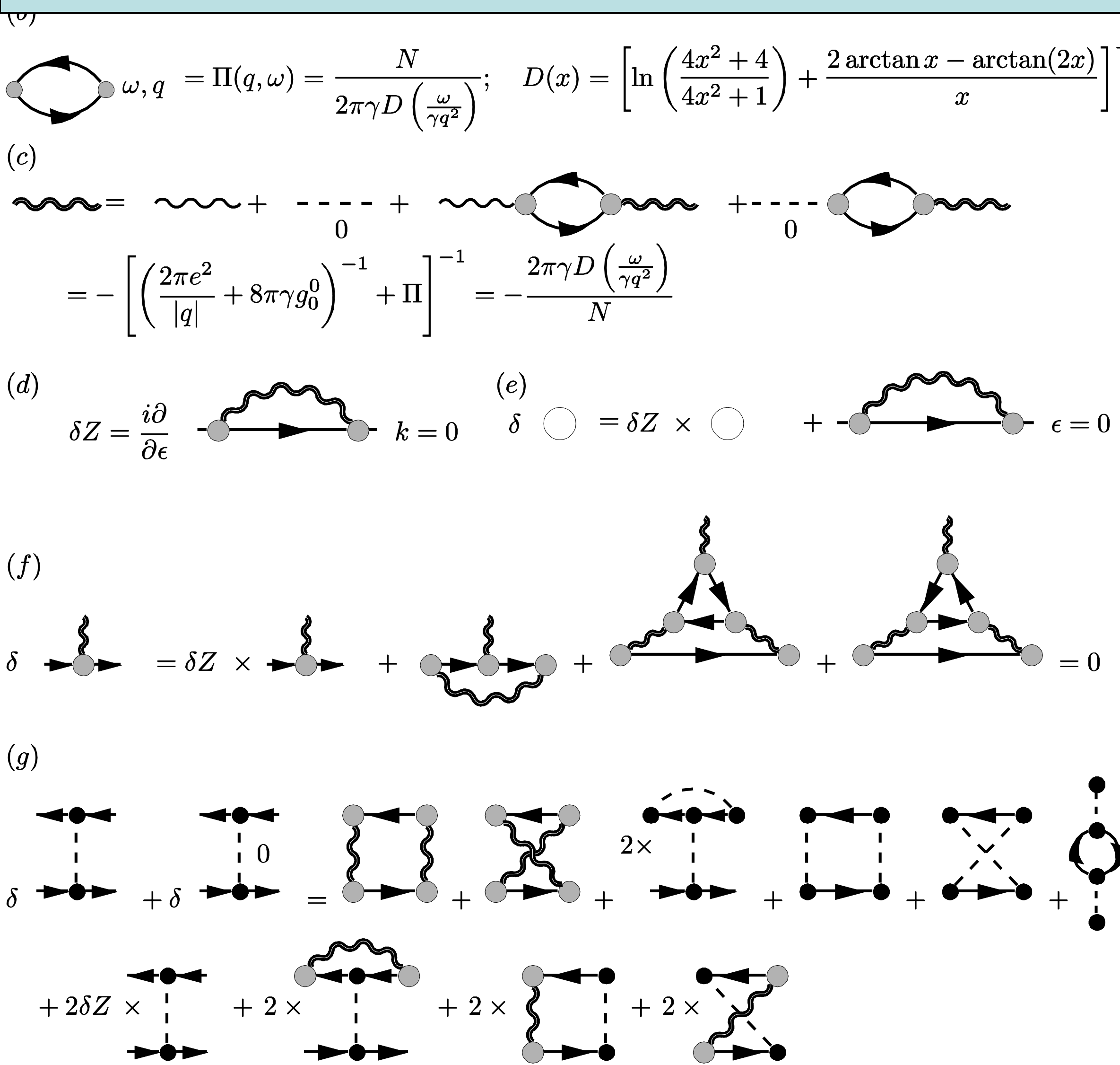
First loop RG

_1/N RG_

Renormalization Group

- ***Iteratively remove highest energy electrons***
- ***Incorporate their effect into redefinition of parameters*** g_{ij} ***&*** m
- ***Parameters become functions of energy scale***
- ***Effectively re-sums logarithmic corrections to observable quantities.***

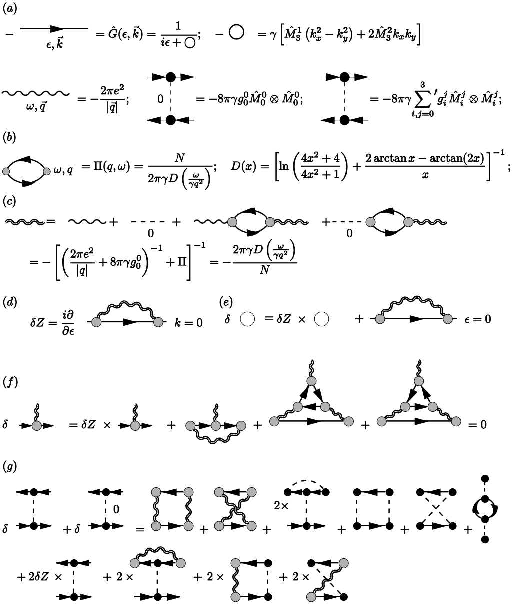
Warning:
1) Each diagram is infrared divergent: only their sum is logarithmic;



Screening of scalar potential

Spectrum curvature renormalization

Short range interaction renormalization



Renormalization Group equations:

$$\frac{dg_{ij}}{d\ell} = -\frac{\alpha_3}{N^2}\delta(E_2)_{ij} - \frac{\alpha_1 + 2\alpha_2 A_{ij}}{N} g_{ij} - \sum_{kl}^{\sim} \frac{g_{kl}}{N}\alpha_2 B_{ij}^{kl} - 2N A_{ij} g_{ij}^2 + \sum_{kl}^{\sim}\sum_{mn}^{\sim} C_{klmn}^{ij} g_{kl} g_{mn}$$

$$\frac{d\log m}{d\ell} = -\frac{\alpha_1}{2N} \approx .01$$

$$\ell \equiv \log(\frac{p_0}{p})$$

Valid only for weak coupling $g_i \ll \frac{1}{N}$

$$A_{ij} \equiv \frac{1}{16}\sum_{\gamma=x,y} tr\left(\left[\hat{\tau}_i^{KK'}\hat{\tau}_j^{AB}, \hat{\tau}_z^{KK'}\hat{\tau}_\gamma^{AB}\right]^2\right)$$

$$B_{kl}^{ij} \equiv \frac{1}{64}\sum_{\gamma=x,y} tr\left(\hat{\tau}_k^{KK'}\hat{\tau}_l^{AB}\left\{\hat{\tau}_i^{KK'}\hat{\tau}_j^{AB}, \hat{\tau}_z^{KK'}\hat{\tau}_\gamma^{AB}\right\}\right)^2$$

$$\alpha_1 \equiv \frac{1}{2\pi}\int dx\, f(x)(1-3x^2)/(1+x^2)^3 \approx .-078$$

$$\alpha_2 \equiv \int \frac{dx}{2\pi} f(x)\frac{2}{(1+x^2)^2} \approx .469$$

$$\alpha_3 \equiv \int \frac{dx}{2\pi}\frac{f(x)^2}{4(1+x^2)^2} \approx .066$$

$$C_{klmn}^{ij} = \frac{1}{8}\sum_{\gamma=x,y} tr\left(\hat{\tau}_k^{KK'}\hat{\tau}_l^{AB}\hat{\tau}_i^{KK'}\hat{\tau}_j^{AB}\hat{\tau}_z^{KK'}\hat{\tau}_\gamma^{AB} \times \left[\hat{\tau}_k^{KK'}\hat{\tau}_l^{AB}, \hat{\tau}_z^{KK'}\hat{\tau}_\gamma^{AB}\right]\hat{\tau}_i^{KK'}\hat{\tau}_j^{AB}\right)$$
$$+\frac{1}{64}\sum_{\gamma=x,y}\left\{tr\left(\hat{\tau}_i^{KK'}\hat{\tau}_j^{AB}\left[\hat{\tau}_k^{KK'}\hat{\tau}_l^{AB}\hat{\tau}_z^{KK'}\hat{\tau}_\gamma^{AB}\hat{\tau}_m^{KK'}\hat{\tau}_n^{AB} + \hat{\tau}_k^{KK'}\hat{\tau}_l^{AB}\hat{\tau}_z^{KK'}\hat{\tau}_\gamma^{AB}\hat{\tau}_m^{KK'}\hat{\tau}_n^{AB}\right]\right)\right\}^2$$
$$+\frac{1}{32}\left\{tr\left(\hat{\tau}_i^{KK'}\hat{\tau}_j^{AB}\left[\hat{\tau}_k^{KK'}\hat{\tau}_l^{AB}, \hat{\tau}_m^{KK'}\hat{\tau}_n^{AB}\right]\right)\right\}^2$$

Analysis of the RG equations:

$$g_i(0) = 0$$

$$\frac{dg_{E_2}(\ell)}{d\ell} = -\frac{1}{N(N+2)}\left(\frac{\alpha_3(N+2)}{N} - \frac{(\alpha_2-\alpha_1)^2}{8N}\right) - 2(N+2)\left(g_{E_2} - \frac{\alpha_2-\alpha_1}{4N(N+2)}\right)^2$$

No fixed point.

It suggests phase transition to nematic phase.

But what happens when $g_i(0) \neq 0$?

RG flow from $g_i(0) = 0$ not stable!
Need to consider full RG equations.

$$\frac{dg_{ij}}{d\ell} = -\frac{\alpha_3}{N^2}\delta(E_2)_{ij} - \frac{\alpha_1 + 2\alpha_2 A_{ij}}{N} g_{ij} - \sum_{kl}^{\sim} \frac{g_{kl}}{N}\alpha_2 B_{ij}^{kl} - 2N A_{ij} g_{ij}^2 + \sum_{kl}^{\sim}\sum_{mn}^{\sim} C_{klmn}^{ij} g_{kl} g_{mn}$$

No fixed points; couplings always diverge at finite energy scale.

Always spontaneously broken symmetry.

Twenty-Six Candidate Phases

8 Singlet	9 Magnetic	9 Superconducting
$\langle \psi^\dagger \tau_i^{KK'} \tau_j^{AB} \psi \rangle$	$\langle \psi^\dagger \tau_i^{KK'} \tau_j^{AB} \vec{\sigma} \psi \rangle$	$\langle \psi^\dagger \tau_i^{KK'} \tau_j^{AB} \hat{\mathcal{T}} \psi^\dagger \rangle$

Mean Field Theory

$$H_{MF} \equiv \sum_k \Psi(\vec{k})^\dagger \Big[\frac{1}{2m} \tau_z^{PH} \tau_z^{KK'} \left(\tau_+^{AB} \hat{p}_+^2 - \tau_-^{AB} \hat{p}_-^2 \right) - \sum_t \left(c_t \mathcal{O}_t \hat{M}^t \right) \Big] \Psi(\vec{k}) + \frac{1}{2} \sum_t c_t \mathcal{O}_t^2$$

$$c_t \equiv \sum_s g_s \left\{ \delta_{st} - \frac{1}{4N^2} tr \left[\left(\hat{M}^s \hat{M}^t \right)^2 \right] \right\}$$

BCS logarithms already incorporated in constants

Competing exchange energy contributions

$$E_{AF} \propto -4g_G - g_{B_2} + 2g_{E_2''} + 2g_{E_2} + 2g_{E_1''} - g_{A_2} + 2g_{E_1} - g_{B_1}$$

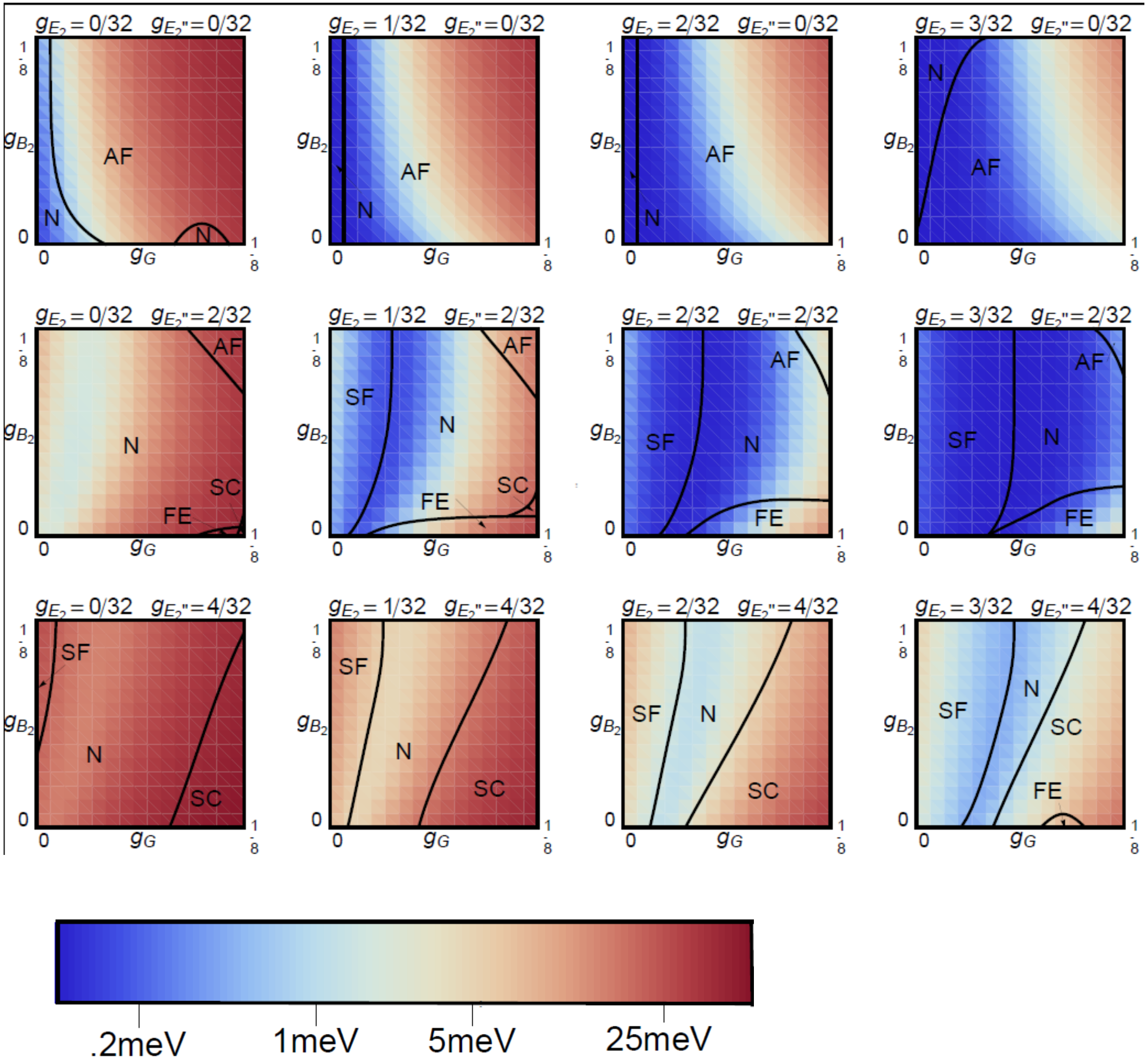
We don't know the values of the bare couplings!

What's reasonable?

- ***Bare couplings small: less than 1/N***
- ***Current-current couplings zero***
- $g_{B_2}\left(\psi^\dagger \tau_z^{AB} \tau_z^{KK'} \psi\right)^2$, $g_G\left(\psi^\dagger \tau_{x,y}^{AB} \tau_{x,y}^{KK'} \psi\right)^2$ ***are dipole-dipole interactions and likely positive.***

Broadly explore parameter space

Results:



AF – Antiferromagnetic

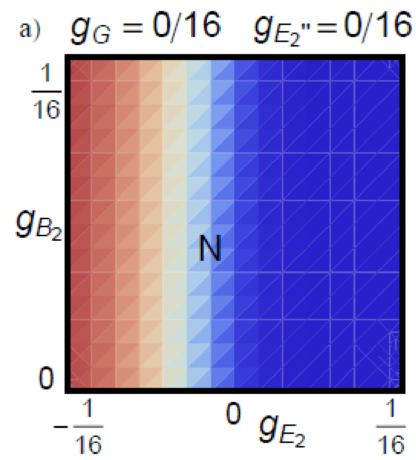
N – Nematic

SF – Spin Flux

FE – Ferroelectric

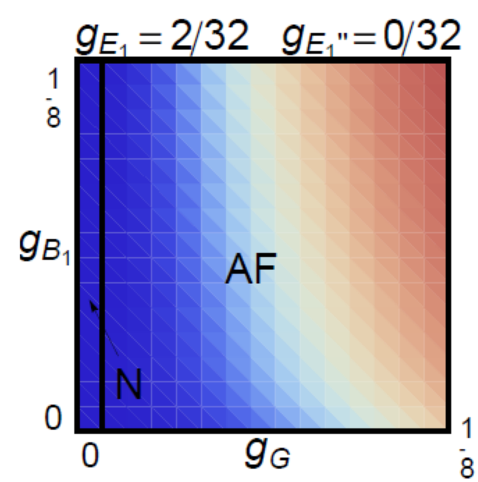
SC – Triplet Superconductor

Without intervalley scattering only nematic phase!



Complex behavior

- $g_{B_2}\left(\psi^\dagger \tau_z^{AB}\tau_z^{KK'}\psi\right)^2$ ***does not introduce AF, but term*** $g_G\left(\psi^\dagger \tau_{x,y}^{AB}\tau_{x,y}^{KK'}\psi\right)^2$ ***does.***
- ***"Current-current" couplings important***
- ***Multiple instabilities in RG flow***

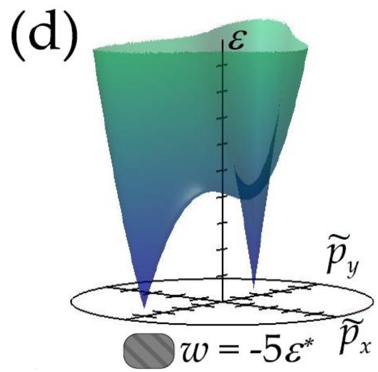


Phases

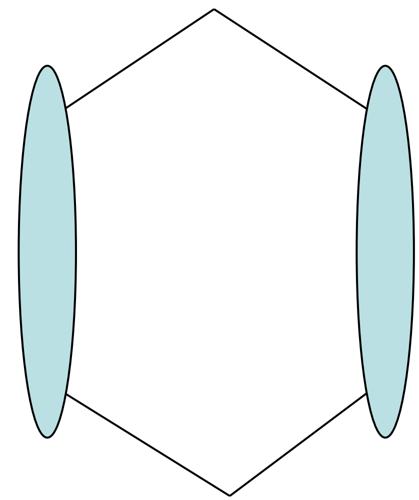
Nematic

$$\langle \psi^\dagger \tau_z^{K\bar{K}'} \tau_{x,y}^{AB} \psi \rangle$$

- Order parameter selects one of BLG's principal axes; akin to uniaxial strain
- Gapless spectrum; parabolic band touching reconstructed.
- Interesting interaction with strain, trigonal warping.
- Discussed by Vafek & Yang, Lemonik *et al*.



Reconstructed dispersion

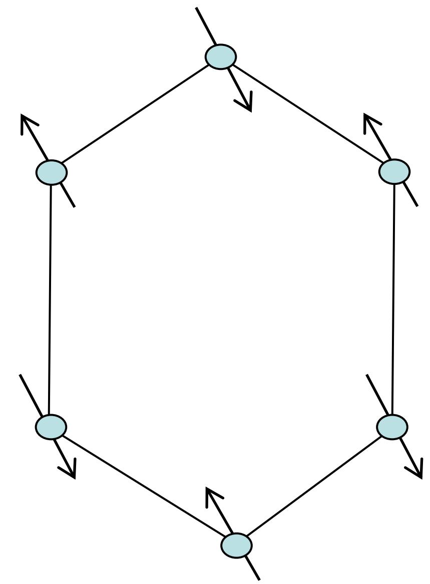


Phases

Antiferromagnetic

$$\langle \psi^\dagger \tau_z^{AB} \tau_z^{KK'} \vec{\sigma} \psi \rangle$$

- Spins oppositely polarized on opposite layers.
- Gapped charge excitations, gapless neutral excitations
- Discussed by Vafek, Kharitonov.

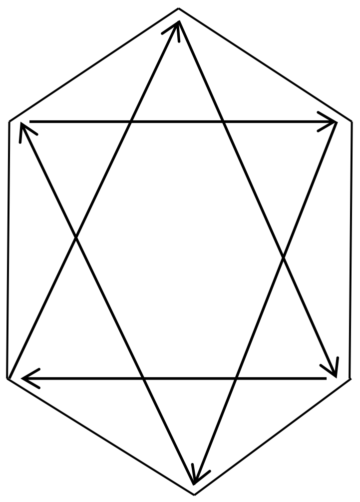


Phases

Spin Flux

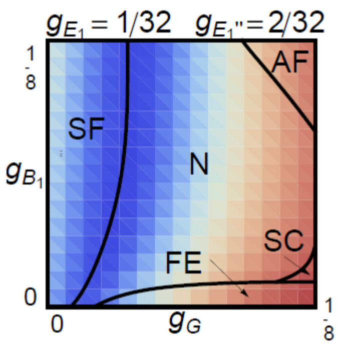
$$\langle \psi^\dagger \bar{\tau}_z^{AB} \vec{\sigma} \psi \rangle$$

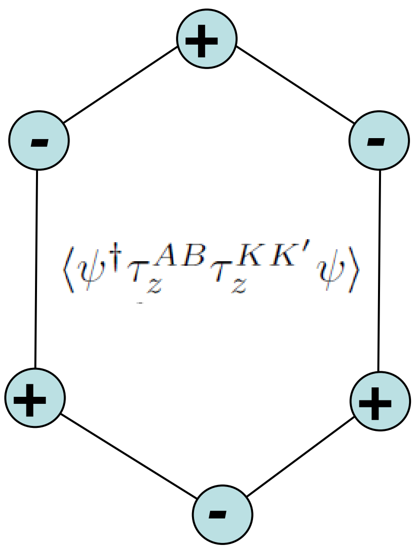
- Persistent spin current circling honeycomb rings
- Gapped charge excitations, gapless neutral excitations
- Quantum spin hall effect?



Least Likely Phases [Fine tuning required]

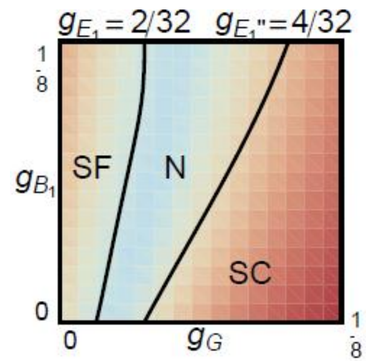
Ferroelectric





$$\langle \psi^\dagger \tau_z^{AB} \tau_z^{KK'} \psi \rangle$$

Triplet Superconductor

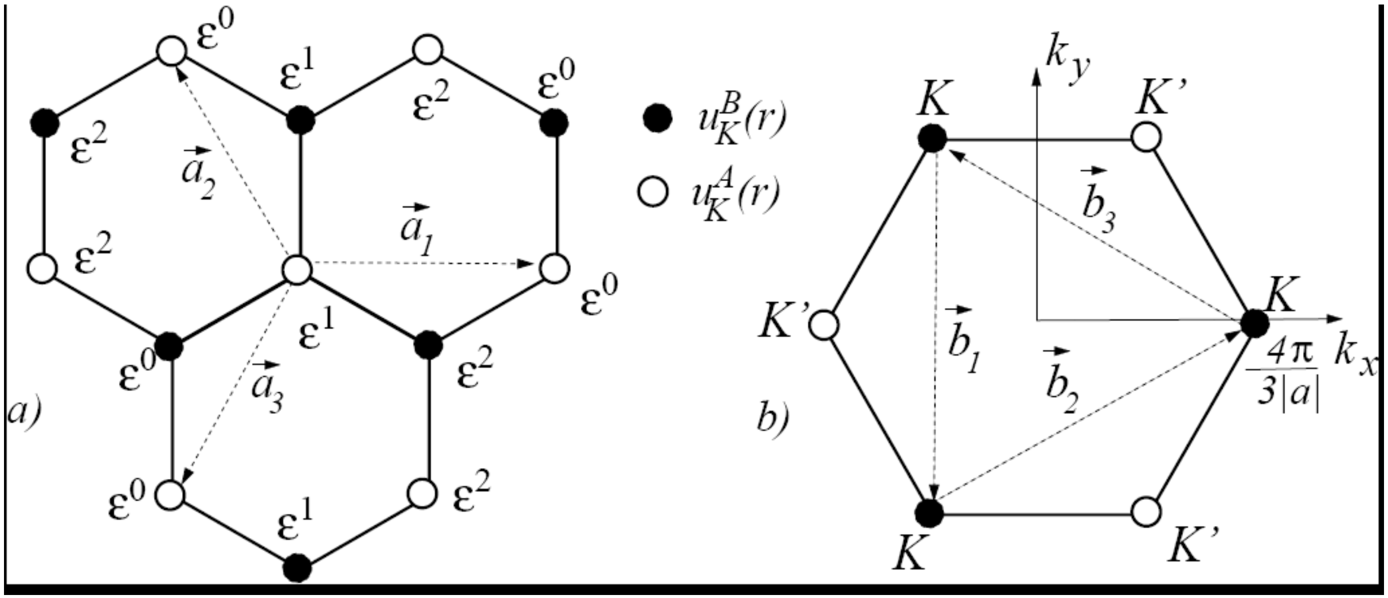


$$\langle \psi^\dagger \tau_z^{KK'} \vec{\sigma} \dot{\mathcal{T}} \psi^\dagger \rangle$$

Conclusions:

- We used 1/N expansion & RG analysis of interaction constants in all symmetry allowed interaction channels to determine possible ground states of BLG: Antiferromagnetic, Nematic, Spin Flux, Superconducting, Ferroelectric.
- Because of instabilities in the RG flow the relation between bare constants & phases is not transparent, sometimes counter-intuitive.
- **Possible strain-induced transition from AF to nematic state**.

Field theory parametrization for bilayer graphene



$$\Psi_s(\mathbf{r};\tau) = \vec{\psi}_s(\mathbf{r},\tau) * \vec{u}(\mathbf{r});\ \ s = \uparrow, \downarrow$$

$$\vec{u} = \begin{pmatrix} \begin{pmatrix} u_K^A \\ u_K^B \end{pmatrix}_{AB} \\ \begin{pmatrix} u_{K'}^B \\ -u_{K'}^A \end{pmatrix}_{AB} \end{pmatrix}_{KK'}$$

Time reversal symmetry:

$$\psi^\dagger \mathcal{H} \psi = \left[\hat{\mathcal{T}} \psi^\dagger\right] \mathcal{H}^T \hat{\mathcal{T}} \psi$$

$$\hat{\mathcal{T}} \equiv i\sigma_y \otimes \tau_y^{AB} \otimes \tau_y^{KK'}$$

- ***Nonlinear differential equation in eight variables.***
- ***Multiple regimes, competing asymptotics.***
- ***No "good" subset of parameters***
- ***Asymptotic behavior of RG when new symmetries emerge is outside domain of applicability of RG equations.***

$$\frac{dg_{ij}}{d\ell} = -\frac{\alpha_3}{N^2}\delta(E_2)_{ij} - \frac{\alpha_1 + 2\alpha_2 A_{ij}}{N} g_{ij} - \tilde{\sum_{kl}} \frac{g_{kl}}{N}\alpha_2 B^{kl}_{ij} - 2NA_{ij}g^2_{ij} + \tilde{\sum_{kl}}\tilde{\sum_{mn}} C^{ij}_{klmn} g_{kl} g_{mn}$$