Theoretical Approach to Many-body Instabilities in Bilayer Graphene

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NATIONAL HIGH MAGNETIC FIELD LAB

Outline:

•Non-interacting (single-body) effects A-B stacked bilayer:

parabolic touching and trigonal warping effects
parabolic touching leads to divergent susceptibilities as T->0

•Many-body interaction effects on the A-B stacked bilayer:

expect ordering even at weak coupling

*Trigonal warping cuts off T->0 singularity, so finite coupling's needed for ordering

Interestingly divergences are in more than one channel => which ordering dominates?

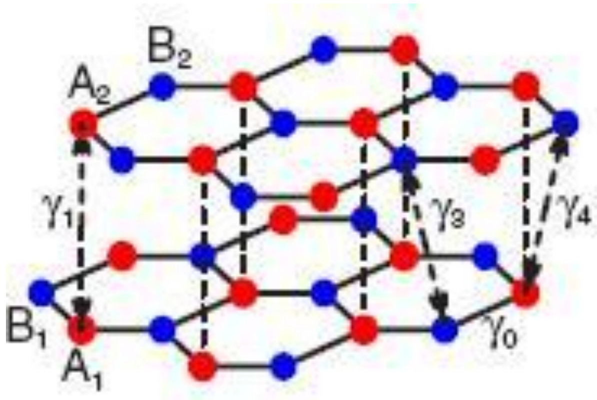
Renormalization group approach:

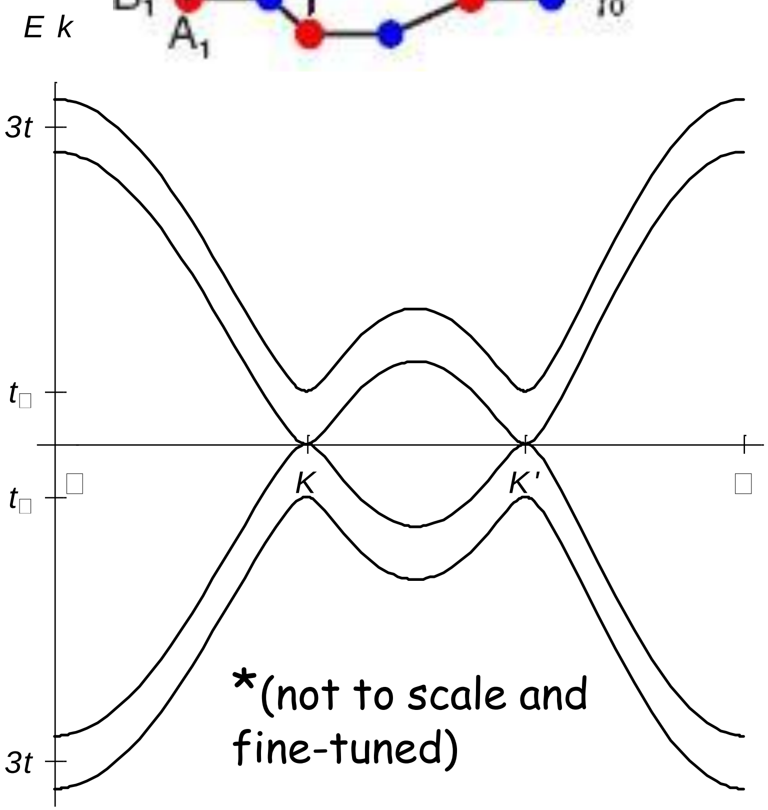
* advantages over self-consistent Hartree-Fock or variational MF

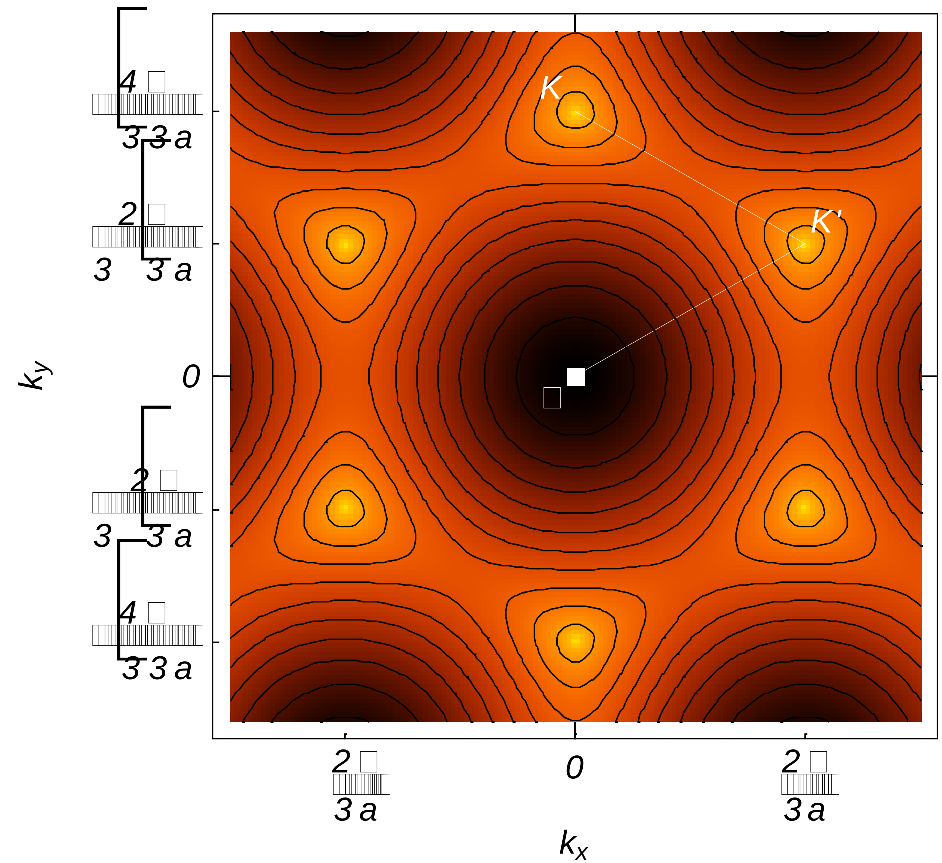
finite range interactions: construct minimal low energy effective field theory
using microscopic symmetry+Fierz reductions

•interaction range >> lattice spacing: electronic nematic
•interaction range ~ lattice spacing i.e. Hubbard model: Neel AF
•how to interpolate between the two limits (work with Robert Throckmorton)

Single-particle physics on bilayer graphene

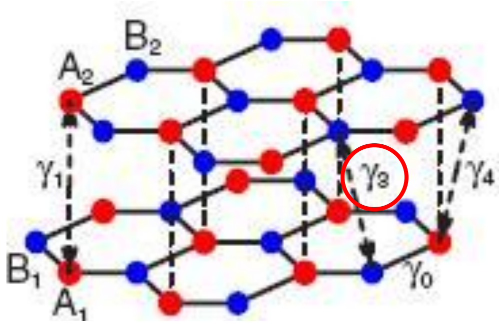




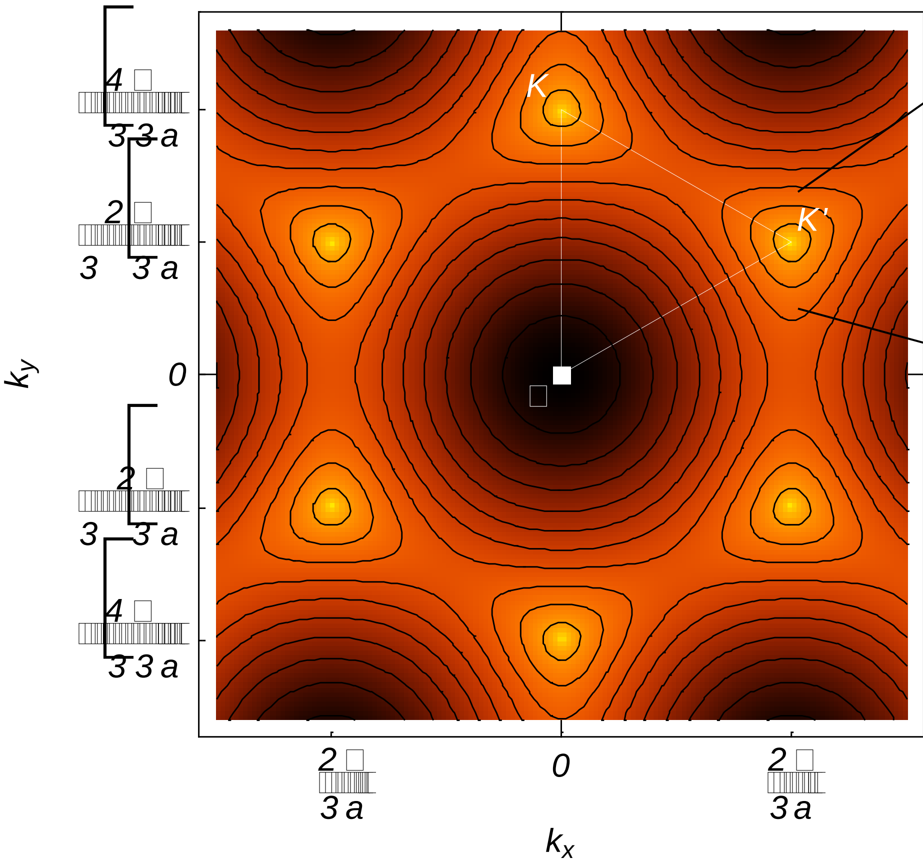


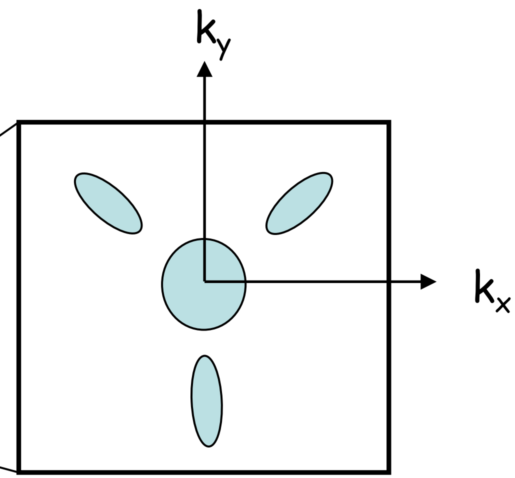
(see e.g. McCann and Falko PRL 2006, Castro Neto et.al. RMP 2009)

Single-particle physics on bilayer graphene: Trigonal warping



$2\pi = (\pi+\pi+\pi)-\pi$





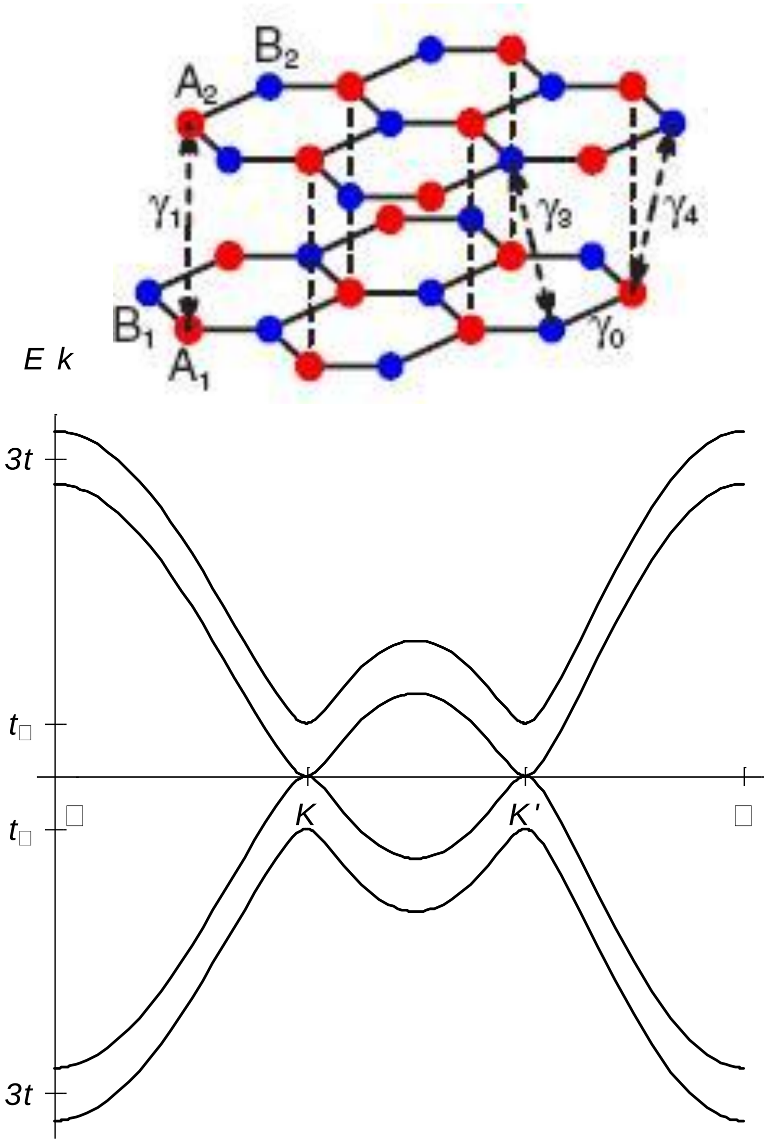
(Anisotropic) massless Dirac fermions

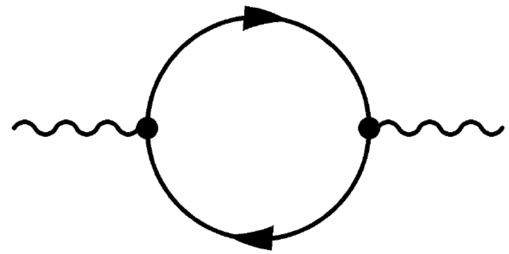
(stable at (very) weak coupling)

$$\frac{\varepsilon_{trig}}{t_\perp} \simeq 10^{-3} - 10^{-2}$$

(see e.g. McCann and Falko PRL 2006)

Ordering susceptibilities on bilayer graphene: motivation





$$\sim \ln\left(t_{\perp}/T\right)$$

- The ordering susceptibility diverges as T->0 in several channels(!) even in the non-interacting limit

- Trigonal warping cuts-off the infra-red singularity so, strictly, ordering is expected only at finite coupling

- Approach: Fine tuning, i.e. ignoring trig. warping, allows controlled access to strong coupling phases from weak coupling

Theory

▪H. Min, G. Borghi, M. Polini, and A. H. MacDonald, Phys. Rev. B **77**, 041407 (2008)
Layer Polarized State (mean field)

▪A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, Rev. Mod. Phys. **81** , 109 (2009).
AF (in strong coupling Hubbard model)

▪O. Vafek and K. Yang, Phys. Rev. B **81** , 041401 (2010).
nematic in weak coupling, when forward scattering dominates

▪F. Zhang, H. Min, M. Polini, and A. H. MacDonald, Phys. Rev. B **81** , 041402 (2010).
inversion symmetry breaking

▪R. Nandkishore and L. Levitov, Phys. Rev. Lett. **104**, 156803 (2010).
QAH

▪Y. Lemonik, I. Aleiner, C. Toke, and V. Fal'ko, Phys. Rev. B 82, 201408(R) (2010)
nematic, weak coupling, attempt at treating the long range part of Coulomb

▪O. Vafek, Phys. Rev. B 82, 205106 (2010)
full treatment of weak coupling spinless, weak coupling Hubbard model

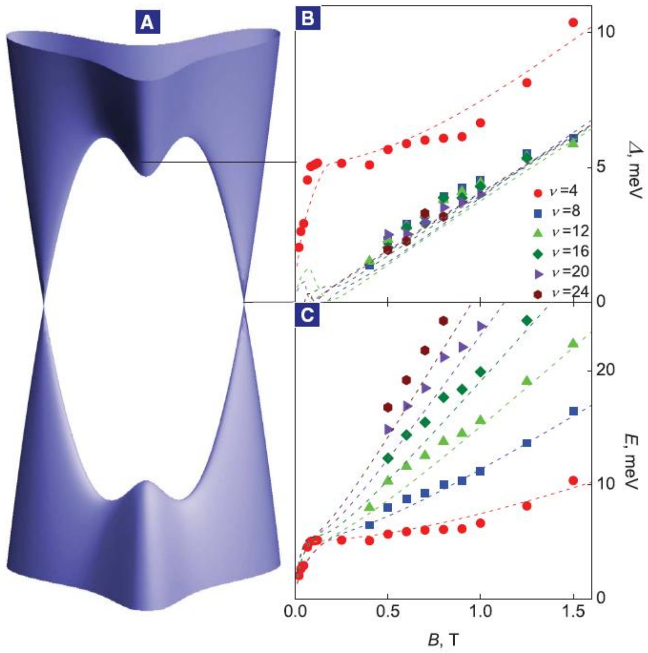
▪J. Jung, F. Zhang A. H. MacDonald, Phys. Rev. B 83, 115408 (2011)
Mean field
…

Experiment:

- R. T. Weitz,et.al., Science **330**, 812 (2010);
 J. Martin, et.al., PRL **105**, 256806 (2010);
Gapless based on transport, with inverse compressibility peaks

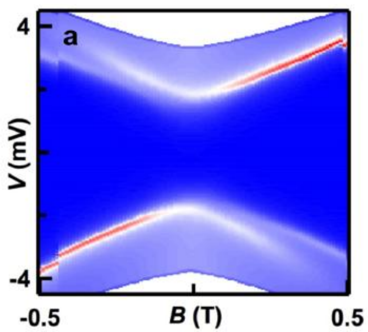
- A. S. Mayorov, et.al. *Science 12 August (2011)*

gapless nematic



- Velasco et.al. arXiv:1108.1609

gap



- Freitag et.al. arXiv:1104.3816

Heuristic (uncontrolled) approach

Not advocated here!

■Variational mean-field: pick a symmetry breaking term, add and subract it from the interacting Hamiltonian, and minimize the expectation value of the interaction – symmetry breaking term

minimize:

■Why is this unreliable as an approach for determining the leading instability?

Preferably selects higher order diagrams while ignoring others which are of the same order (unlike RG or parquette)

Weak coupling renormalization group approach

Advantages:

✓capable of treating the particle-hole and particle-particle instabilities on equal footing

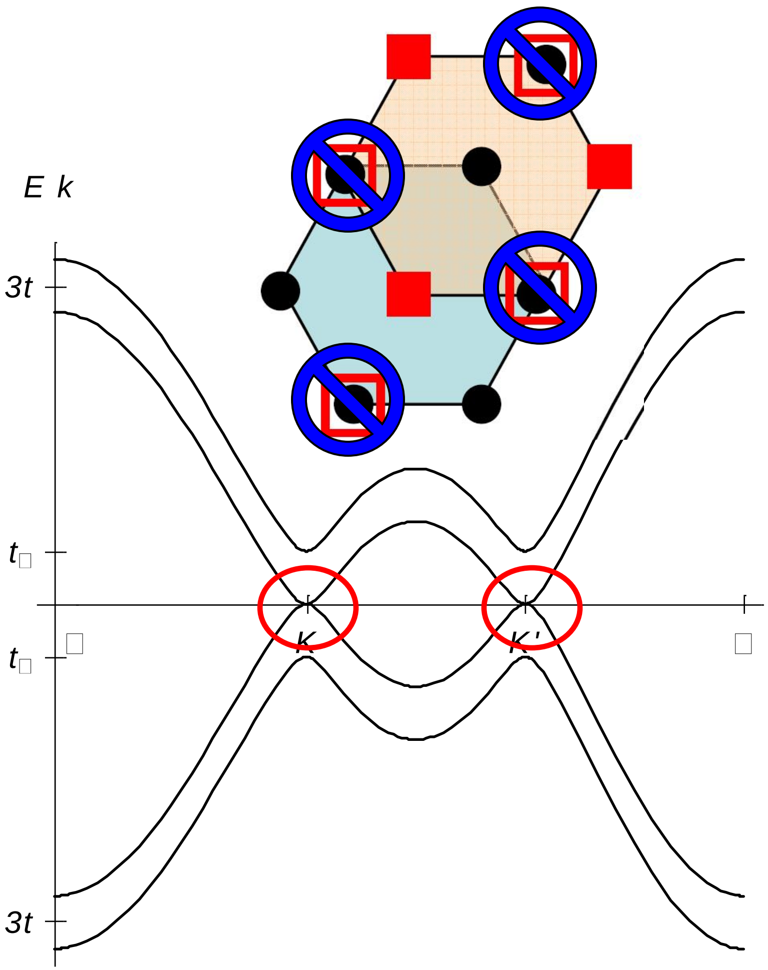
✓capable of correctly resumming leading logarithms at each order in perturbation theory

✓technically doable at weak coupling

OV and Kun Yang, PRB **81**, 041401(R) (2010), (Physics 3, 1 (2010))
OV, PRB **82**, 205106 (2010)
See also Lemonik et.al. PRB 82, 201408(R) (2010).

Construction of the effective low energy field theory

Integrate out the dimerized sites
and high energy modes



$$\mathcal{S}_0 = \int d\tau d^2\mathbf{r} \left[\psi^\dagger \left(\frac{\partial}{\partial \tau} + \sum_{a=x,y} \Sigma^a d^a_{\mathbf{k}} \right) \psi \right]$$

$$d^x_{\mathbf{k}} = \frac{k_x^2 - k_y^2}{2m^*}$$

$$d^y_{\mathbf{k}} = \frac{2k_x k_y}{2m^*}$$

$$\Sigma^x = 1\sigma^x \quad 1_N$$

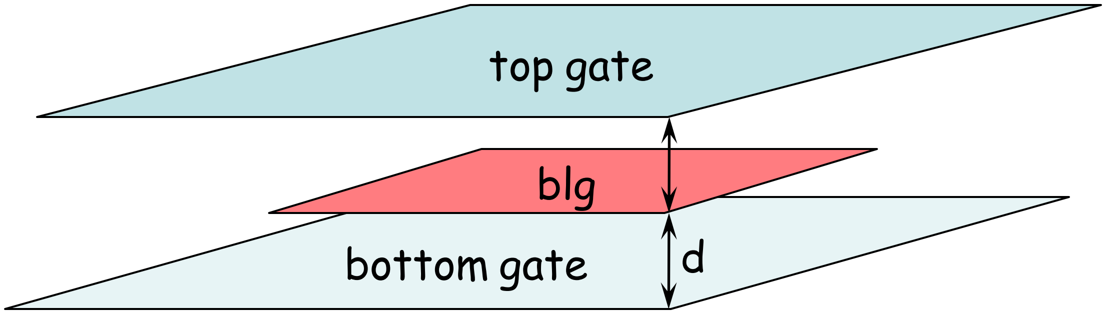
$$\Sigma^y = \tau^z \sigma^y \quad 1_N$$

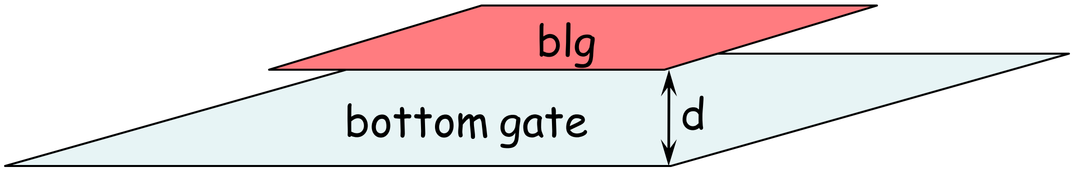
$$\Sigma^z = \tau^z \sigma^z \quad 1_N$$

valley (τ^z) layer (σ^z)

- Scaling z=2 ($\omega \sim k^2$)
- By power counting, contact interactions are the only marginal couplings

Construction of the effective low energy field theory





In both cases the interaction have a finite range: V(q=0) is non-divergent.

Construction of the effective low energy field theory

$$\mathcal{S} = \int d\tau d^2\mathbf{r} \left[\psi^\dagger \left(\frac{\partial}{\partial\tau} + \sum_{a=x,y} \Sigma^a d^a_{\mathbf{k}} \right) \psi \right] + \frac{1}{2} \sum_{ST} g_{ST} \int d\tau d^2\mathbf{r} \psi^\dagger S\psi(\mathbf{r},\tau)\psi^\dagger T\psi(\mathbf{r},\tau)$$

- *S* and *T* are 8x8 matrices (naively 2*136=272 couplings)
- Lattice symmetry x time reversal x spin SU(2)

further reduces the number to 18 for spinful (9 for spinless)

Linear (in)dependence of interaction terms and Fierz identities

Grassmann 8-component field

For x=y this leads to 9 linear constraints on *g*'s, the interaction couplings

bilayer: OV, PRB **82**, 205106 (2010)
spinless single layer: Herbut *et.al.* PRB **79** 085116 (2009)

Short range interactions

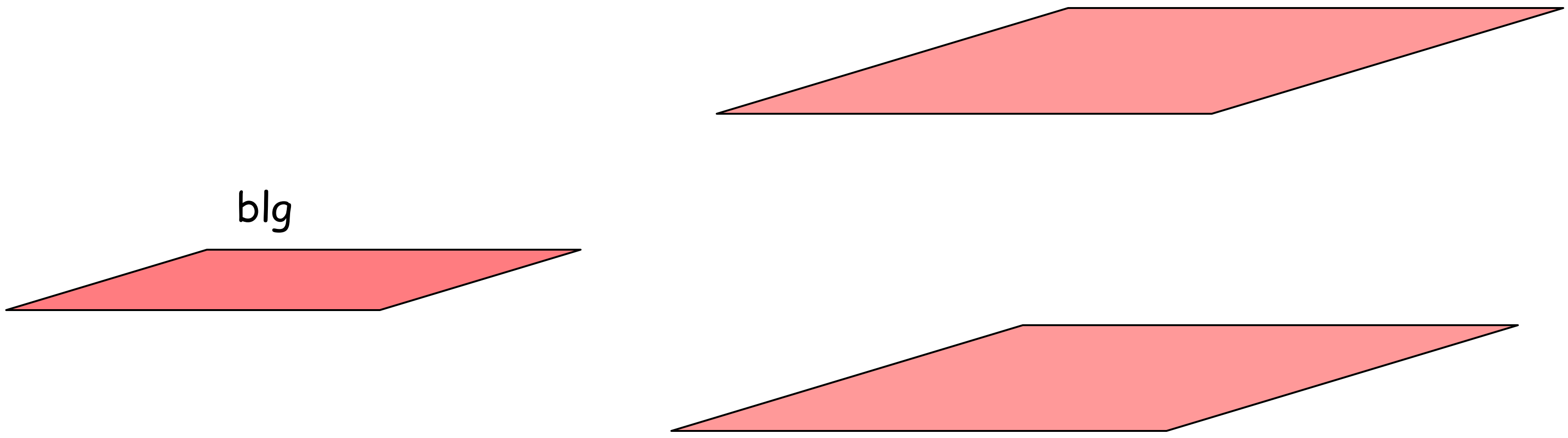
$$
\begin{aligned}
L_{int} &= \frac{1}{2}\int d^2\mathbf{r}\left[g^{(c)}_{A_1}\left(\psi^\dagger A_1\psi(\mathbf{r},\tau)\right)^2 + g^{(c)}_{A_2}\left(\left(\psi^\dagger A_2\psi(\mathbf{r},\tau)\right)^2 + \left(\psi^\dagger D_1\psi(\mathbf{r},\tau)\right)^2\right)\right] \\
&+ \frac{1}{2}\int d^2\mathbf{r}\left[g^{(c)}_{B_1}\left(\left(\psi^\dagger B_1\psi(\mathbf{r},\tau)\right)^2 + \left(\psi^\dagger C_2\psi(\mathbf{r},\tau)\right)^2\right) + g^{(c)}_{B_2}\left(\psi^\dagger B_2\psi(\mathbf{r},\tau)\right)^2\right] \\
&+ \frac{1}{2}\int d^2\mathbf{r}\left[g^{(c)}_{D_2}\left(\psi^\dagger D_2\psi(\mathbf{r},\tau)\right)^2 + g^{(c)}_{\gamma}\left(\left(\psi^\dagger C_3\psi(\mathbf{r},\tau)\right)^2 + \left(\psi^\dagger D_3\psi(\mathbf{r},\tau)\right)^2\right)\right] \\
&+ \frac{1}{2}\int d^2\mathbf{r}\left[g^{(c)}_{C_1}\left(\psi^\dagger C_1\psi(\mathbf{r},\tau)\right)^2 + g^{(c)}_{\alpha}\left(\left(\psi^\dagger A_3\psi(\mathbf{r},\tau)\right)^2 + \left(\psi^\dagger B_3\psi(\mathbf{r},\tau)\right)^2\right)\right] \\
&+ \frac{1}{2}\int d^2\mathbf{r}\left[g^{(c)}_{\beta}\sum_{X=A,B,C,D}\left(\psi^\dagger X_4\psi(\mathbf{r},\tau)\right)^2\right]
\end{aligned}
$$

9-independent couplings

$A_1 = 1_4 \quad 1$	$A_2 = 1\sigma^x \quad 1$ $D_1 = \tau^z\sigma^y \quad 1$	$D_2 = \tau^z\sigma^z \quad 1$	$C_3 = \tau^x\sigma^y \quad 1$ $D_3 = \tau^y\sigma^y \quad 1$
$B_1 = \tau^z\sigma^x \quad 1$ $C_2 = -1\sigma^y \quad 1$	$B_2 = \tau^z 1 \quad 1$	$C_1 = 1\sigma^z \quad 1$	$A_3 = \tau^x\sigma^x \quad 1$ $B_3 = \tau^y\sigma^x \quad 1$
$A_4 = \tau^x 1 \quad 1$	$B_4 = -\tau^y 1 \quad 1$	$C_4 = -\tau^x\sigma^z \quad 1$	$D_4 = -\tau^y\sigma^z \quad 1$

valley layer spin

Microscopic interaction and four-point couplings

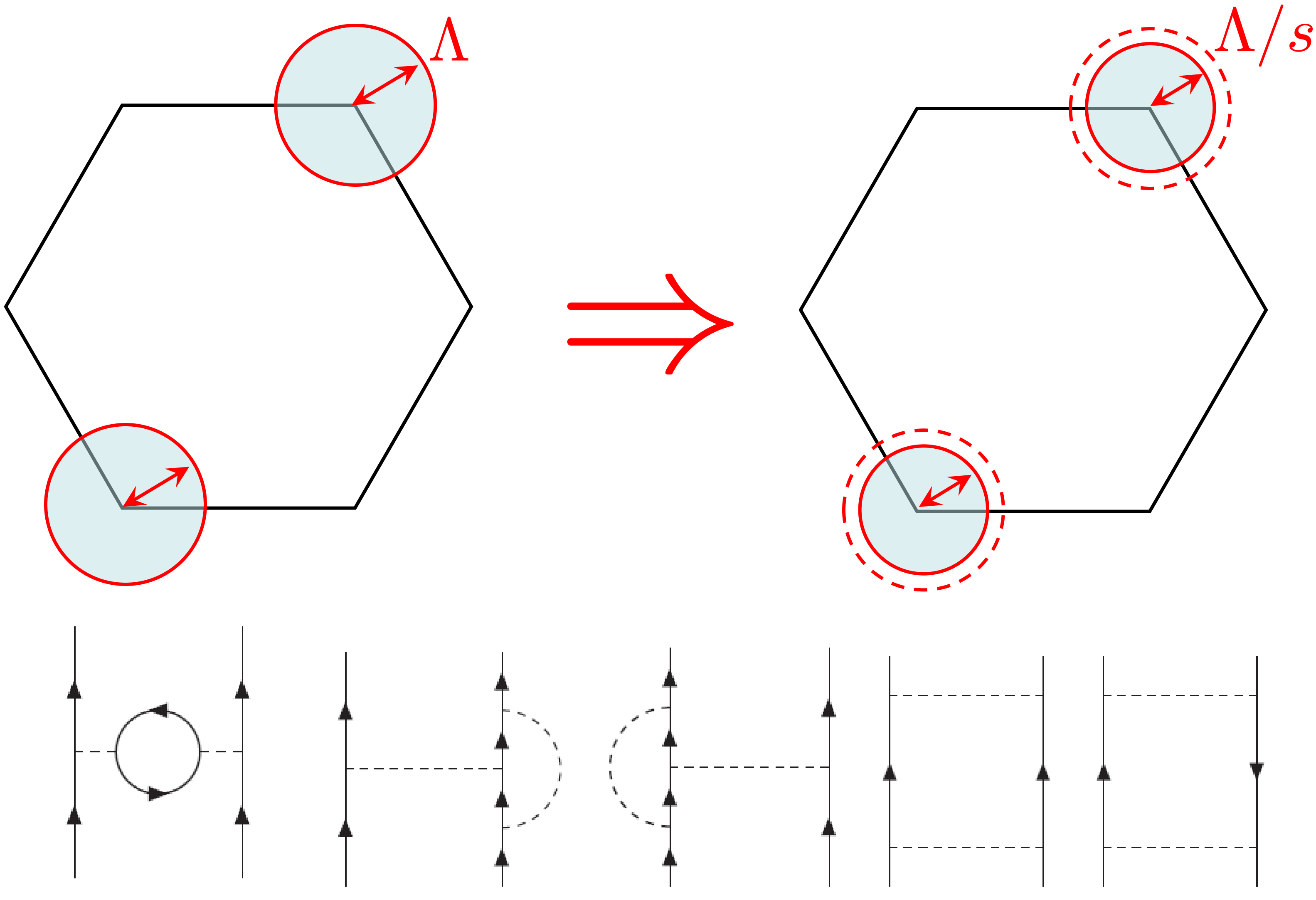


Initial couplings:

*no umklapp (unlike in 1D at ½ filling)

R. E. Throckmorton, OV arXiv:1111.2076

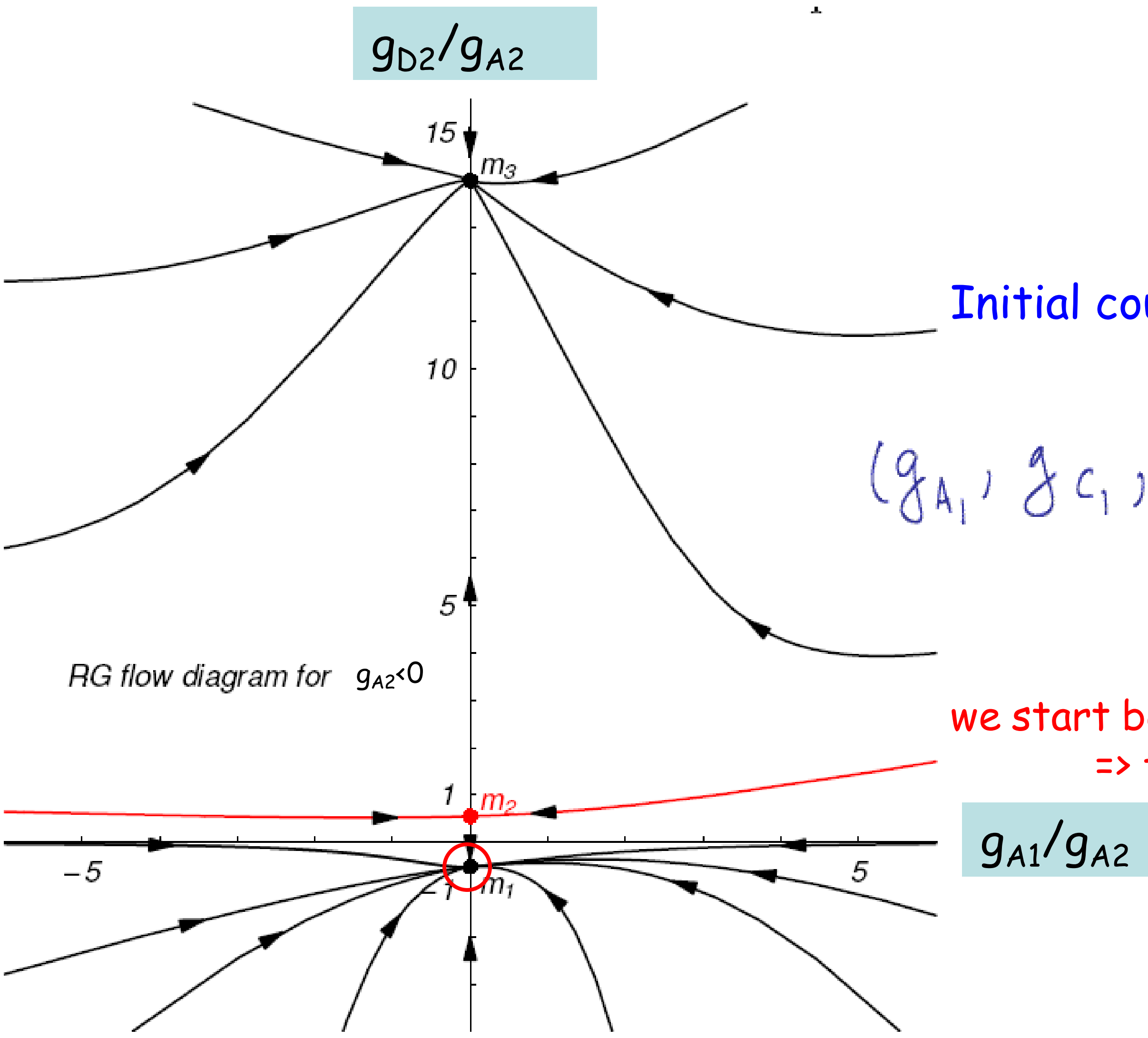
Effective low energy theory: RG procedure



RG equations for the interaction coupling constants

$$
\begin{aligned}
\frac{dg_{A_1}^{(c)}}{d\ln s} &= -4\left(g_{A_1}^{(c)}g_{A_2}^{(c)} + g_{B_1}^{(c)}g_{B_2}^{(c)} + 2g_{\alpha}^{(c)}g_{\beta}^{(c)}\right)\frac{m}{4\pi} \\
\frac{dg_{A_2}^{(c)}}{d\ln s} &= \left(-{g_{A_1}^{(c)}}^2 + 2g_{A_1}^{(c)}g_{A_2}^{(c)} - 12{g_{A_2}^{(c)}}^2 - {g_{B_2}^{(c)}}^2 - (g_{C_1}^{(c)} - 2g_{B_1}^{(c)})^2 - {g_{D_2}^{(c)}}^2 + 2g_{A_2}^{(c)}\left(g_{B_2}^{(c)} - g_{C_1}^{(c)} + g_{D_2}^{(c)} + 2g_{\alpha}^{(c)} - 2g_{\gamma}^{(c)}\right)\right. \\
&- \left. 2\left({g_{\alpha}^{(c)}}^2 + \left(g_{\gamma}^{(c)} - 2g_{\beta}^{(c)}\right)^2\right)\right)\frac{m}{4\pi} \\
\frac{dg_{B_1}^{(c)}}{d\ln s} &= \left(2g_{B_1}^{(c)}\left(g_{A_1}^{(c)} - 4g_{B_1}^{(c)} - 4g_{A_2}^{(c)} + g_{B_2}^{(c)} - g_{C_1}^{(c)} + g_{D_2}^{(c)} - 2g_{\alpha}^{(c)} + 2g_{\gamma}^{(c)}\right)\right. \\
&- \left. 2\left(g_{A_1}^{(c)}g_{B_2}^{(c)} - g_{C_1}^{(c)}(2g_{A_2}^{(c)} - g_{D_2}^{(c)}) - 2g_{\alpha}^{(c)}(2g_{\beta}^{(c)} - g_{\gamma}^{(c)})\right)\right)\frac{m}{4\pi} \\
\frac{dg_{B_2}^{(c)}}{d\ln s} &= -4\left(g_{A_1}^{(c)}g_{B_1}^{(c)} + g_{A_2}^{(c)}g_{B_2}^{(c)} - {g_{\alpha}^{(c)}}^2 - 2{g_{\beta}^{(c)}}^2 + 2g_{\beta}^{(c)}g_{\gamma}^{(c)} - {g_{\gamma}^{(c)}}^2\right)\frac{m}{4\pi} \\
\frac{dg_{C_1}^{(c)}}{d\ln s} &= 4\left(g_{C_1}^{(c)}\left(g_{A_1}^{(c)} - 3g_{A_2}^{(c)} - 2g_{B_1}^{(c)} + g_{B_2}^{(c)} - 3g_{C_1}^{(c)} + g_{D_2}^{(c)} - 2g_{\alpha}^{(c)} + 4g_{\beta}^{(c)} - 2g_{\gamma}^{(c)}\right)\right. \\
&+ \left. g_{B_1}^{(c)}(2g_{A_2}^{(c)} - g_{D_2}^{(c)}) - 2g_{\alpha}^{(c)}(g_{\beta}^{(c)} - g_{\gamma}^{(c)})\right)\frac{m}{4\pi} \\
\frac{dg_{D_2}^{(c)}}{d\ln s} &= 4\left(g_{D_2}^{(c)}\left(g_{A_1}^{(c)} - 3g_{A_2}^{(c)} - 2g_{B_1}^{(c)} + g_{B_2}^{(c)} + g_{C_1}^{(c)} - 3g_{D_2}^{(c)} + 2g_{\alpha}^{(c)} - 4g_{\beta}^{(c)} + 2g_{\gamma}^{(c)}\right)\right. \\
&+ \left. {g_{A_2}^{(c)}}^2 + g_{B_1}^{(c)}\left(g_{B_1}^{(c)} - g_{C_1}^{(c)}\right) + 2g_{\beta}^{(c)}\left(g_{\beta}^{(c)} - g_{\gamma}^{(c)}\right)\right)\frac{m}{4\pi} \\
\frac{dg_{\alpha}^{(c)}}{d\ln s} &= -4\left(g_{\alpha}^{(c)}\left(g_{A_2}^{(c)} - g_{B_2}^{(c)}\right) + g_{\beta}^{(c)}\left(g_{A_1}^{(c)} - 2g_{B_1}^{(c)} + g_{C_1}^{(c)}\right) + g_{\gamma}^{(c)}\left(g_{B_1}^{(c)} - g_{C_1}^{(c)}\right)\right)\frac{m}{4\pi} \\
\frac{dg_{\beta}^{(c)}}{d\ln s} &= 2\left(g_{\beta}^{(c)}\left(g_{A_1}^{(c)} - 4g_{A_2}^{(c)} + g_{B_2}^{(c)} + g_{C_1}^{(c)} + g_{D_2}^{(c)} - 4g_{\beta}^{(c)}\right) - g_{\alpha}^{(c)}\left(g_{A_1}^{(c)} - 2g_{B_1}^{(c)} + g_{C_1}^{(c)}\right) + g_{\gamma}^{(c)}\left(2g_{A_2}^{(c)} - g_{B_2}^{(c)} - g_{D_2}^{(c)}\right)\right)\frac{m}{4\pi} \\
\frac{dg_{\gamma}^{(c)}}{d\ln s} &= -4\left(g_{\alpha}^{(c)}\left(g_{B_1}^{(c)} - g_{C_1}^{(c)}\right) + g_{\beta}^{(c)}\left(g_{B_2}^{(c)} - 2g_{A_2}^{(c)} + g_{D_2}^{(c)}\right) - g_{\gamma}^{(c)}\left(g_{A_1}^{(c)} - 3g_{A_2}^{(c)} + 2g_{B_1}^{(c)} - g_{C_1}^{(c)} + g_{D_2}^{(c)} - 4g_{\gamma}^{(c)}\right)\right)\frac{m}{4\pi}
\end{aligned}
$$

Interaction range >> lattice spacing : RG flow



Initial couplings:

$(g_{A_1}, g_{C_1}, g_{\beta}) = g_1(1, 0, 0)$

we start below the red separatrix
=> flow to m_1

Analysis of the susceptibilities

Introduce additional source terms in the action, which correspond to possible broken symmetry states

$$\Delta \mathcal{S} \quad = \quad -\Delta_{ph}^{\mathcal{O}_i} \int d\tau d^2\mathbf{r} \left[\psi^\dagger \mathcal{O}_i \psi\right] - \Delta_{pp}^{\mathcal{O}_i} \int d\tau d^2\mathbf{r} \left[\psi_{\alpha\sigma} \mathcal{O}^i_{\alpha\beta,\sigma\sigma'} \psi_{\beta\sigma'}\right]$$

The question of instability is answered by finding Δ with the strongest RG divergence.

particle-hole channel

(32 terms)

$$\mathcal{O}_i = \tau^\mu \sigma^\nu \quad 1 \text{ or } \mathcal{O}_i = \tau^\mu \sigma^\nu \quad \vec{\sigma},$$

$$\Delta_{ph,ren} \quad = \quad \Delta_{ph} \left(1 + \left[\sum_{j=1}^{9} A_j g_j\right] \frac{m}{4\pi} \ln s\right)$$

pairing channel

(6 triplet+10 singlet)

$$\psi_{\alpha\sigma} \mathcal{O}^{(i)}_{\alpha\beta} \psi_{\beta\sigma'}$$

$$\Delta^{\tau^\mu\sigma^\nu}_{pp,ren} \quad = \quad \Delta_{pp} \left(1 + \left[\sum_{j=1}^{9} A'_j g_j\right] \frac{m}{4\pi} \ln s\right)$$

Most dominant instability: Interaction range >> lattice spacing

Starting with screened Coulomb interaction only, the strongest divergence is found for the operators

$$\boxed{\psi^\dagger 1\sigma_x \quad 1\psi(\mathbf{r}) \text{ and } \psi^\dagger \tau_z\sigma_y \quad 1\psi(\mathbf{r})}$$

This corresponds to an electronic nematic state:

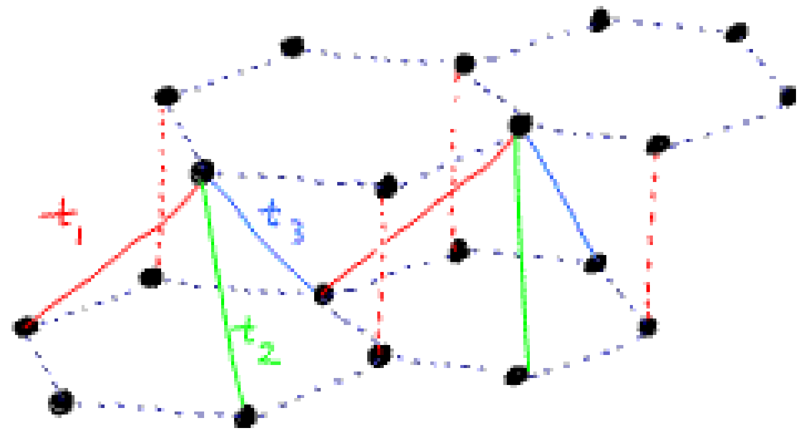
- Breaks rotational symmetry
- Even under π rotation
- Does not break translational symmetry (unlike stripes)

OV and Kun Yang, **PRB 81**, 041401(R) (2010)
subsequently corroborated by Lemonik et.al. PRB 82, 201408(R) (2010).

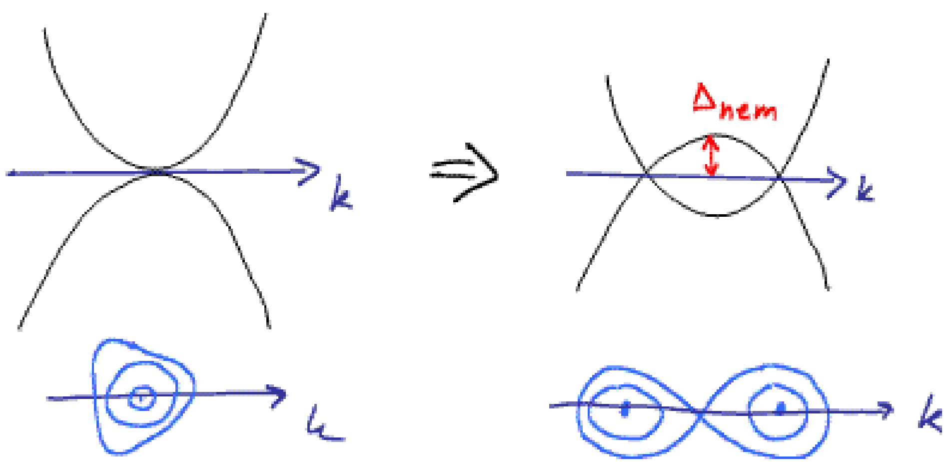
Interaction range >> lattice spacing: Nematic

Starting with screened Coulomb interaction only, the strongest divergence is found for the operators

$$\psi^\dagger 1\sigma_x \quad 1\psi(\mathbf{r}) \text{ and } \psi^\dagger \tau_z\sigma_y \quad 1\psi(\mathbf{r})$$

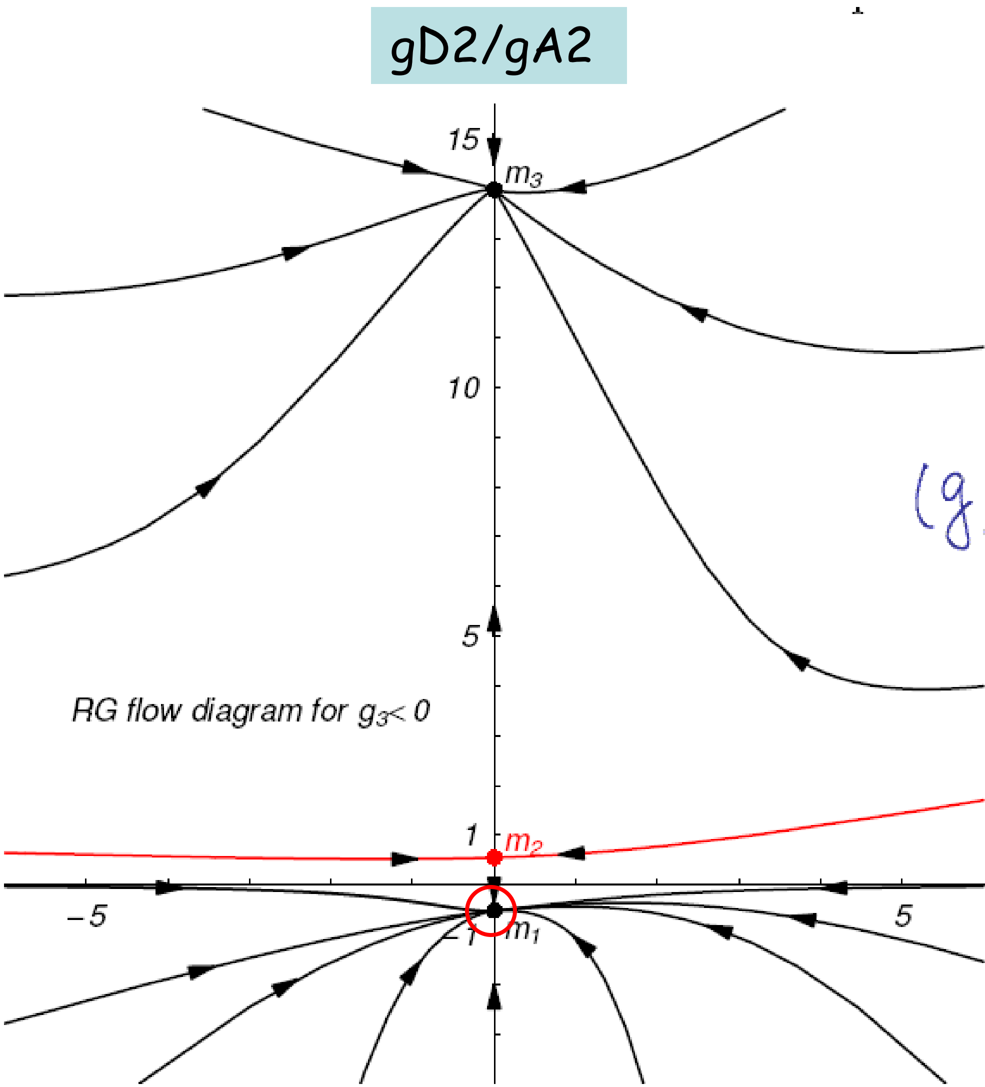


Each parabolic touching is split into two conical (Dirac) points.



Experimental signatures reported in Mayorov et.al. Science Aug 2011

Digression: Interaction range >> lattice spacing



Initial couplings:

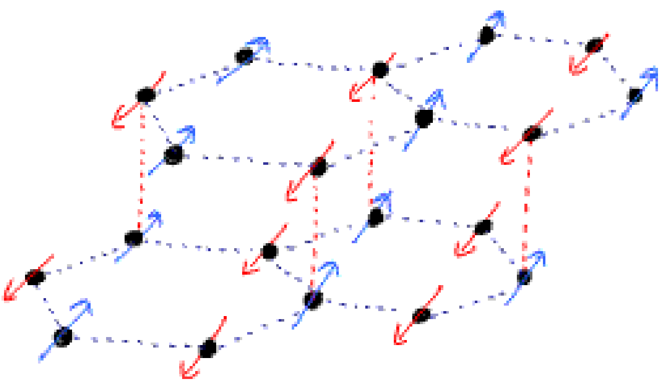
$$(g_{A_1}, g_{C_1}, g_{\beta}) = g_1(1, 0, 0)$$

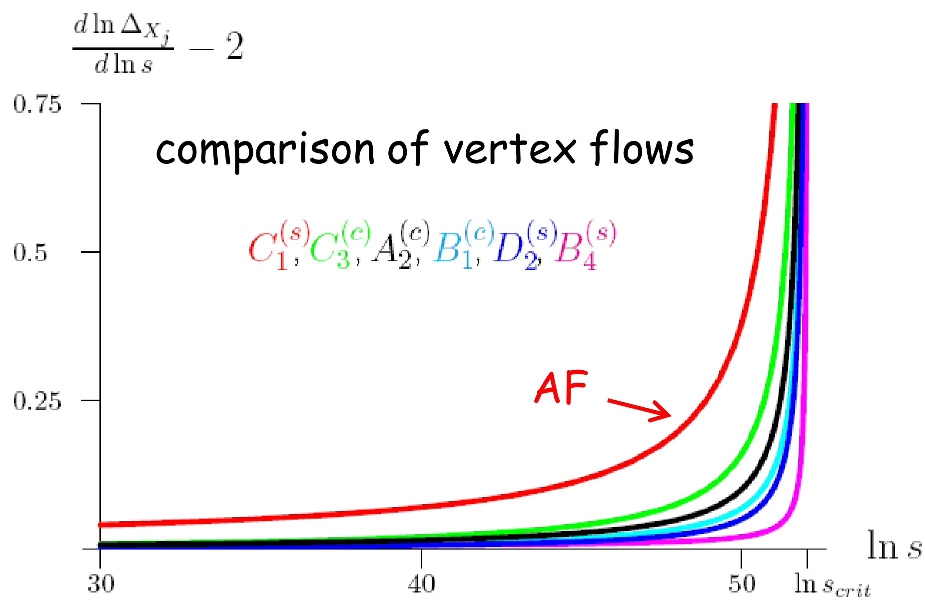
we start below the red separatrix
=> flow to m1

Interaction range ~ lattice spacing:
Repulsive Hubbard model

Strong coupling: bilayer Heisenberg model, not frustrated -> Neel AF

Weak coupling: initially $(g_{A_1}, g_{C_1}, g_\beta) = g_1(1, 1, \frac{1}{2})$



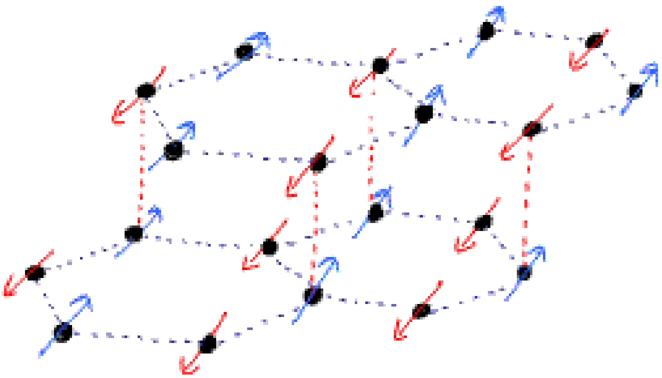


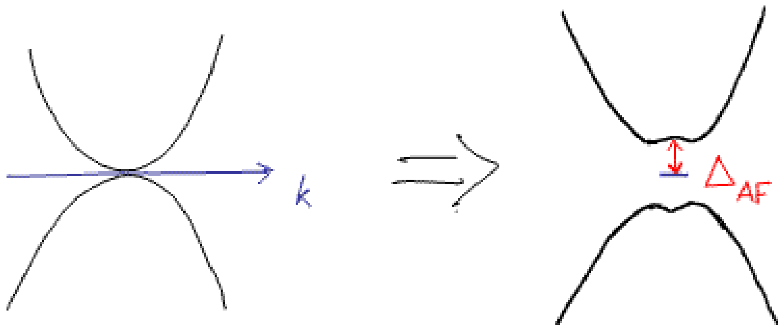
OV, PRB **82**, 205106 (2010)

Interaction range ~ lattice spacing: Repulsive Hubbard model

Strong coupling: bilayer Heisenberg model, not frustrated -> Neel AF

Weak coupling:





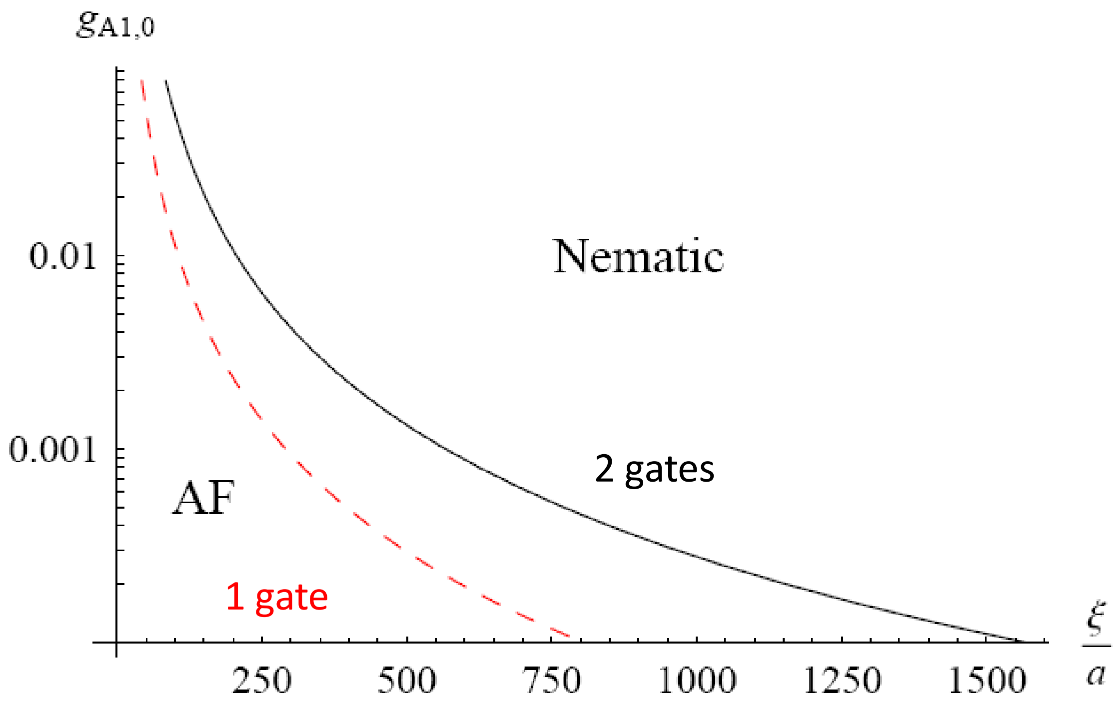
For Neel AF single particle spectrum is gapped

Consistent with experimental results of Velasco et.al .

Phase diagram as a function of the interaction range

nature of the broken symmetry state in BLG depends on the range ξ of the repulsive interaction

Phase diagram (from numerical integration of RG eqs.)



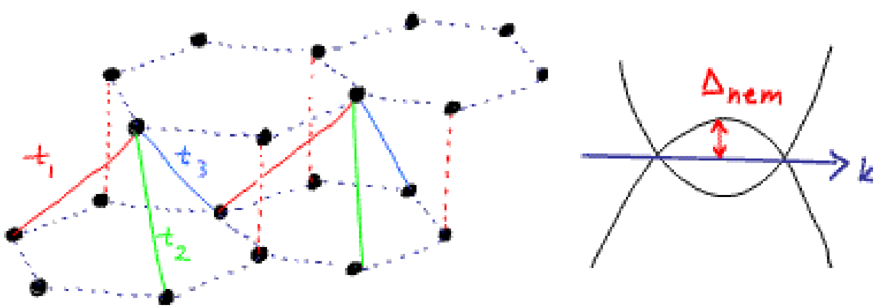
R. E. Throckmorton, OV arXiv:1111.2076 + Robert's KITP poster

Conclusions

SLG: •a critical strength of e-e interaction must be exceeded for a phase transition into a different phase to occur for both short and long range Coulomb interactions
•still, there are interesting renormalization effects on the semi-metal side.

BLG: •Interactions need not be too large to cause a phase transition
•nature of the broken symmetry state in BLG depends on the range ξ of the repulsive interaction

Forward scattering dominates



appreciable 2K scattering