FRG approaches to graphene - an overview

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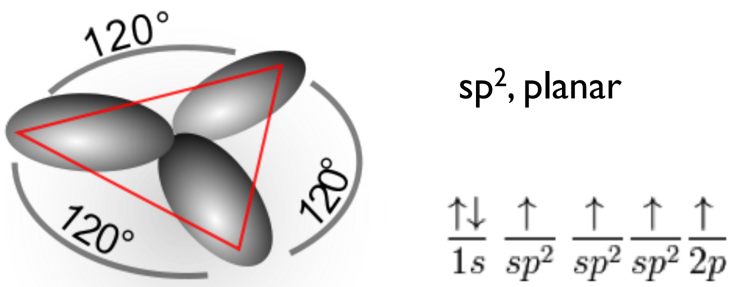
Outline

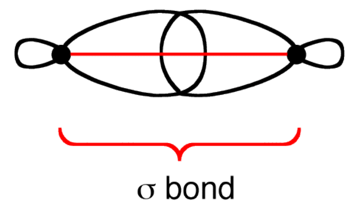
- **Part I: Graphene basics**
- **Part II: Instabilities and phase transitions from (F)RG**
    - **undoped graphene**, Dirac electrons
    - **doped graphene** @van-Hove singularity
- **Conclusions & Outlook**

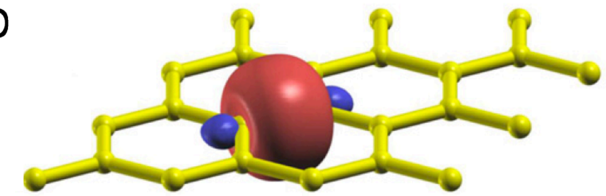
Real space structure

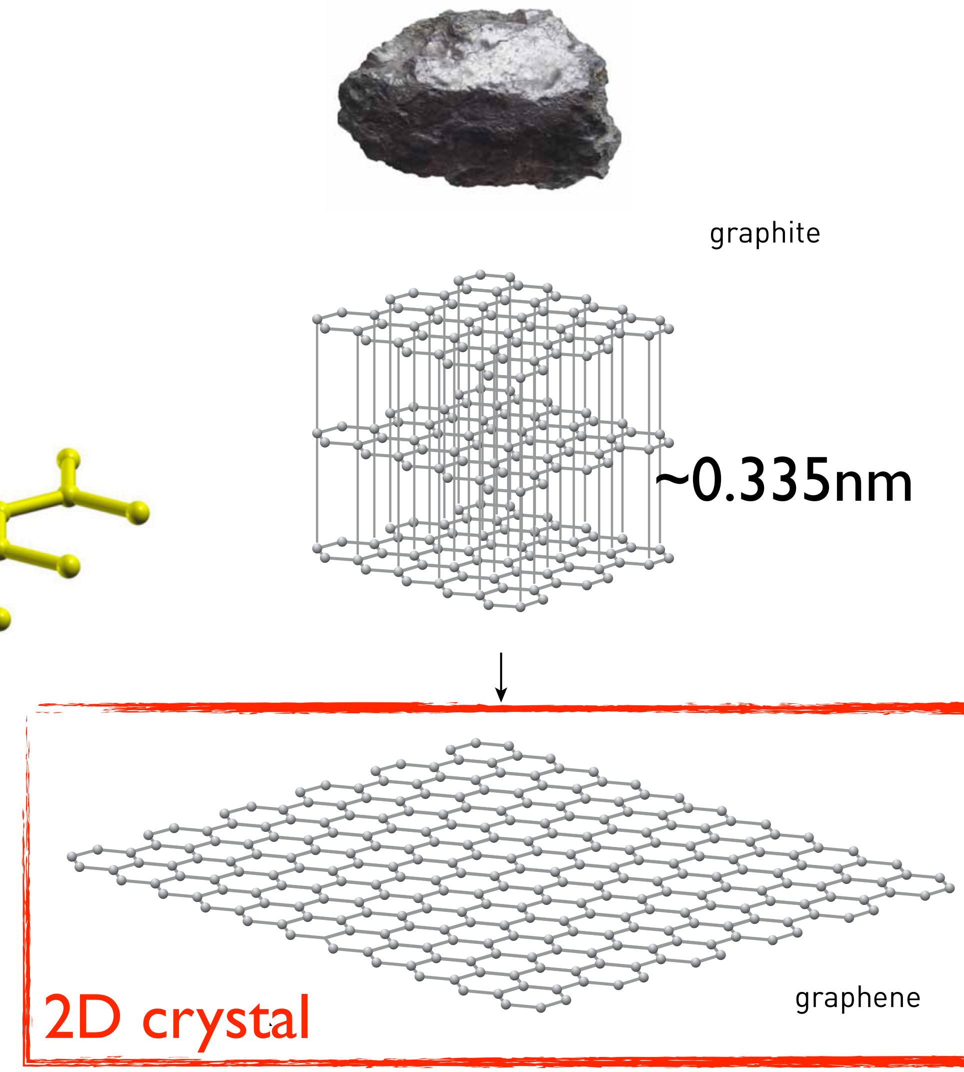
- Graphene: flat single layer of C-atoms in 2D hexagonal lattice

- sp^2-Hybrid-orbitals of C-atoms → σ-bonds away from ϵ_F

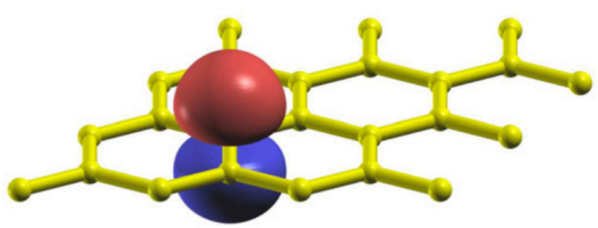


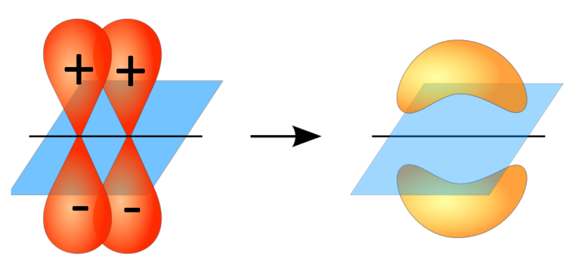






- Conduction & valence e^-: π-bonds of p_z-orbitals



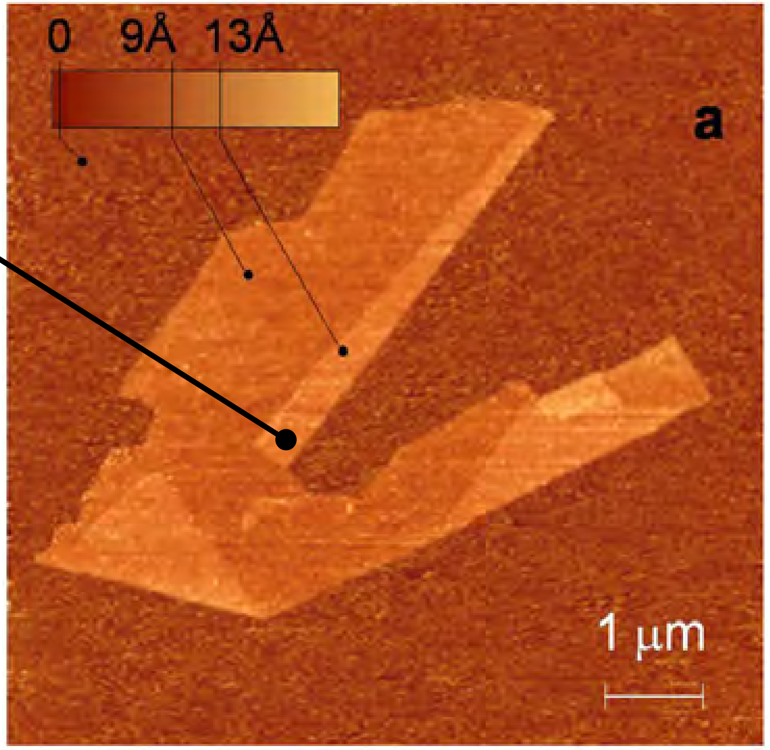


- Van der Waal's bonds between layers

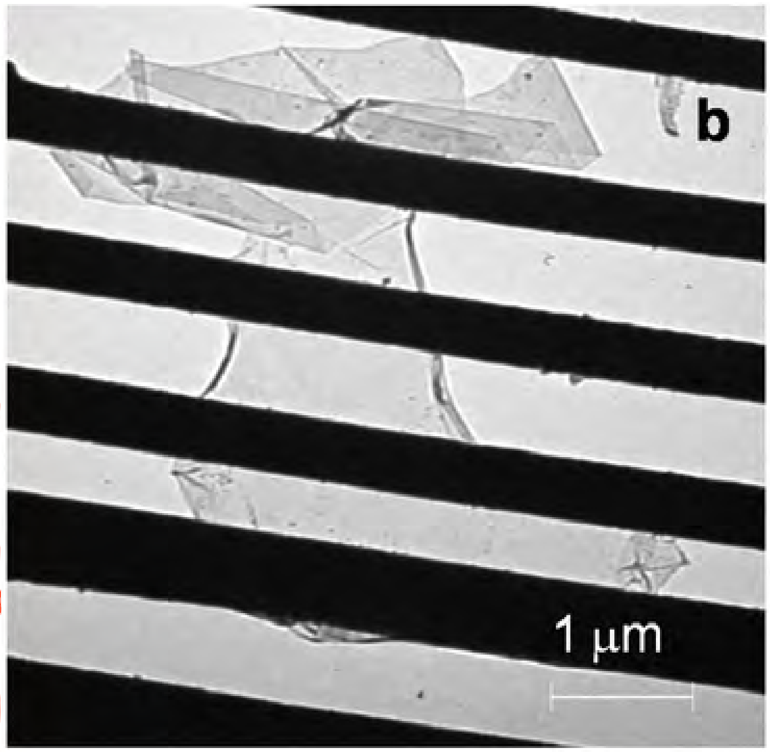
In the lab

Atomic-force microscopy

rel. height ~ 0.4nm
→ single layer

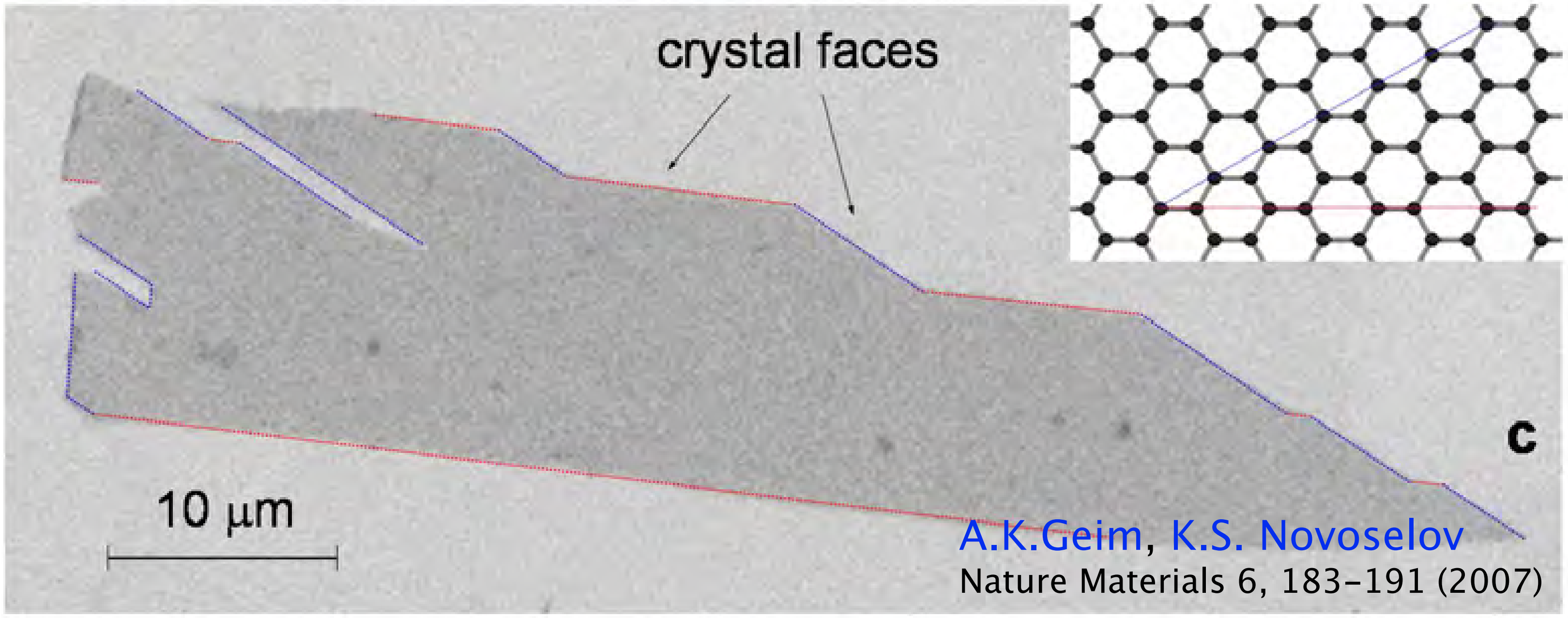


Transmission-electron spectroscopy



suspended on scaffold

large flake



A.K.Geim, K.S. Novoselov
Nature Materials 6, 183-191 (2007)

Scanning-electron micrograph

Fun facts

- **Density**: 0.77mg/m^2
  - even the smallest gas atom (He) cannot pass through it
- **Optical transparency**:
  - Absorbs only 2.3% of the visible light intensity
- **Strength**: breaking strength=42N/m.
  - Thin film of steel (0.335nm) has 2D breaking strength ~0.3N/m

- **Electrical conductivity**: as well as copper
  - 2D sheet conductivity $\sigma = e\ n\ \mu$
    - high electron mobility μ, weakly depends on T even at ~ 300K
    - mobility remains high even in doped devices → in contrast to bulk semiconductors

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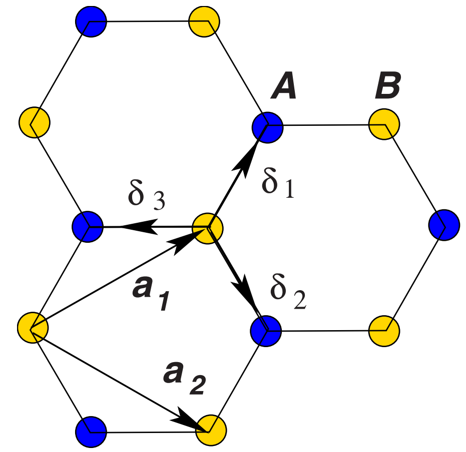
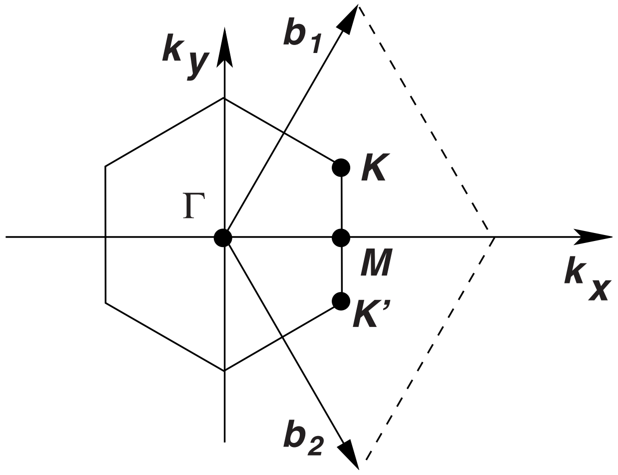
Tight-binding model

$$H_0 = -\,t \sum_{\langle i,j\rangle,\sigma} \left(a^\dagger_{i,\sigma} b_{j,\sigma} + \text{H.c.}\right) - t' \sum_{\langle\langle i,j\rangle\rangle,\sigma} \left(a^\dagger_{i,\sigma} a_{j,\sigma} + b^\dagger_{i,\sigma} b_{j,\sigma} + \text{H.c.}\right)$$



Brillouin zone



- π band structure of graphene: $E_\pm(\mathbf{k}) = \pm t\sqrt{3 + f(\mathbf{k})} - t' f(\mathbf{k})$, $\quad f(\mathbf{k}) = \sum_{i=1}^{3} e^{i\delta_i \cdot \mathbf{k}}$

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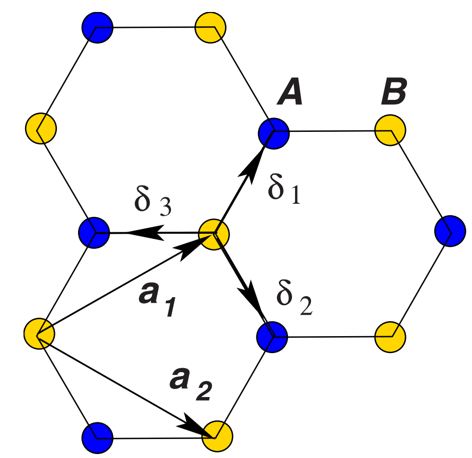
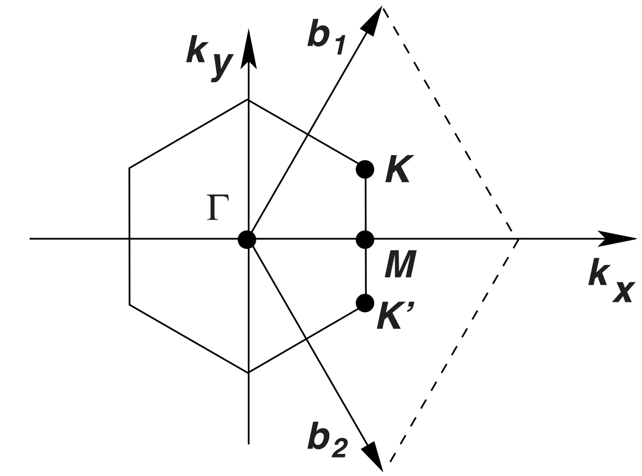


Brillouin zone



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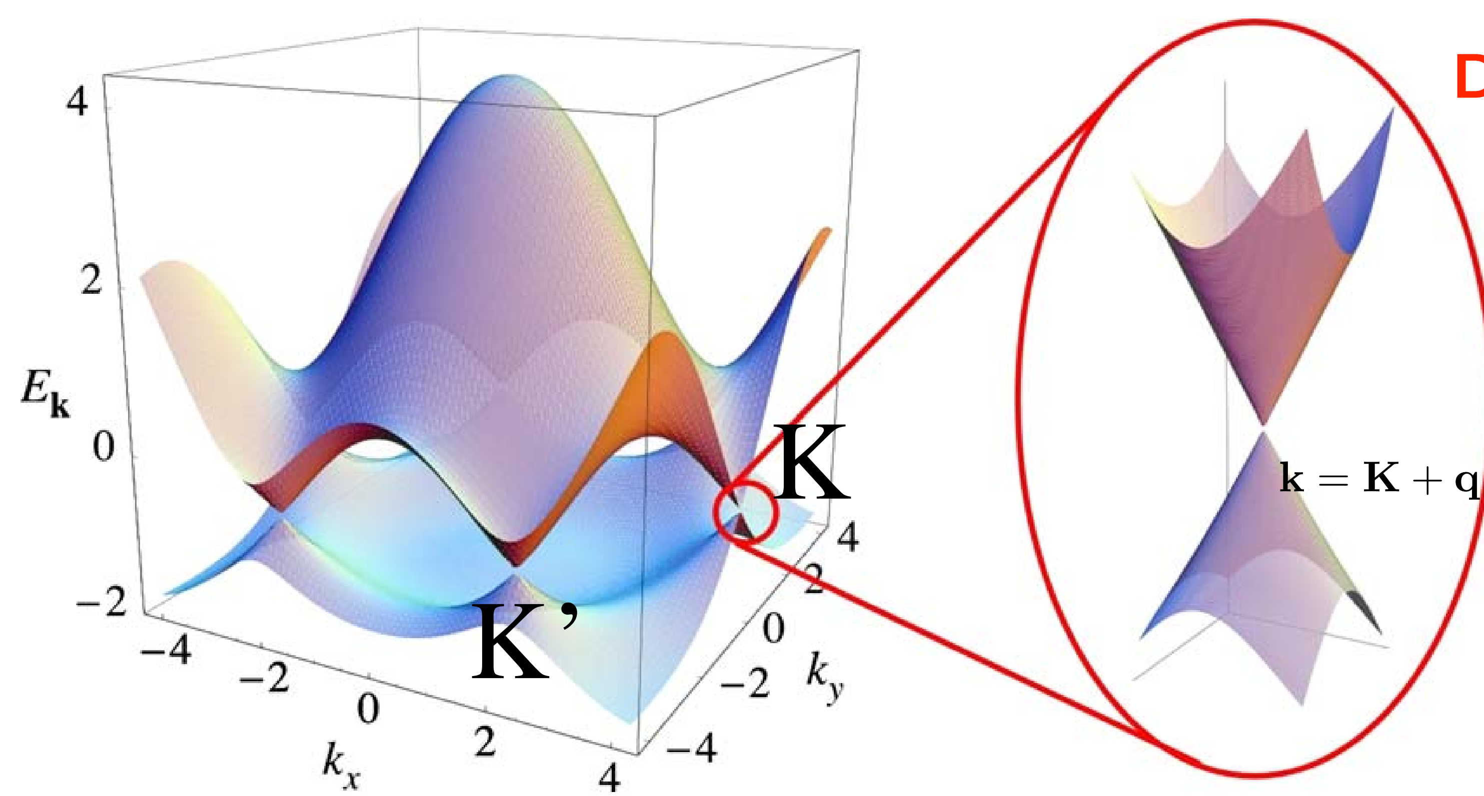
- e.g. from *ab initio* calculations: $t = 2.8\ \mathrm{eV}, t' = -0.2t$

Dirac point



$$E_\pm(\mathbf{q}) \approx 3t' \pm v_F|\mathbf{q}|$$

- adjust Fermi level by chemical potential → **doping**

Castro Neto et al, Rev. Mod. Phys. **81**, 109 (2009)

Dirac fermions in undoped graphene

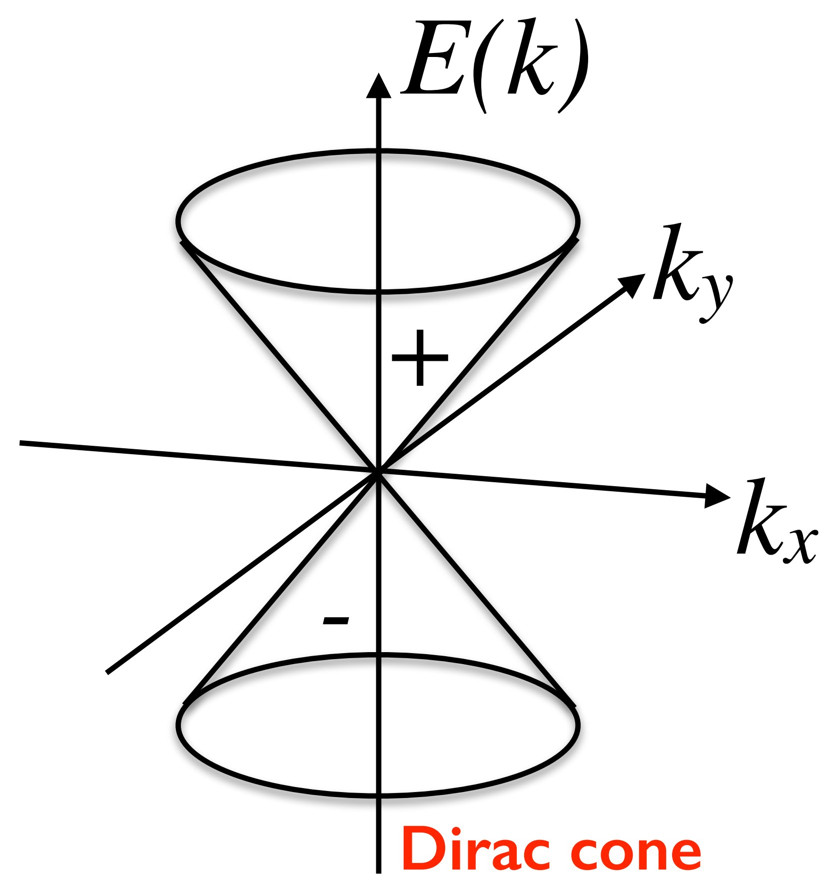
- Expand operators in Hamiltonian around Fermi level → K, K' points
  - **2D massless Dirac equation (around K point)**:

$$-iv_F\vec{\sigma}\cdot\nabla\psi(\vec{r}) = E\psi(\vec{r})$$

  - near Dirac point electrons have well-defined **chirality**

include K' point

➡ **two copies of massless Dirac-like Hamiltonian**

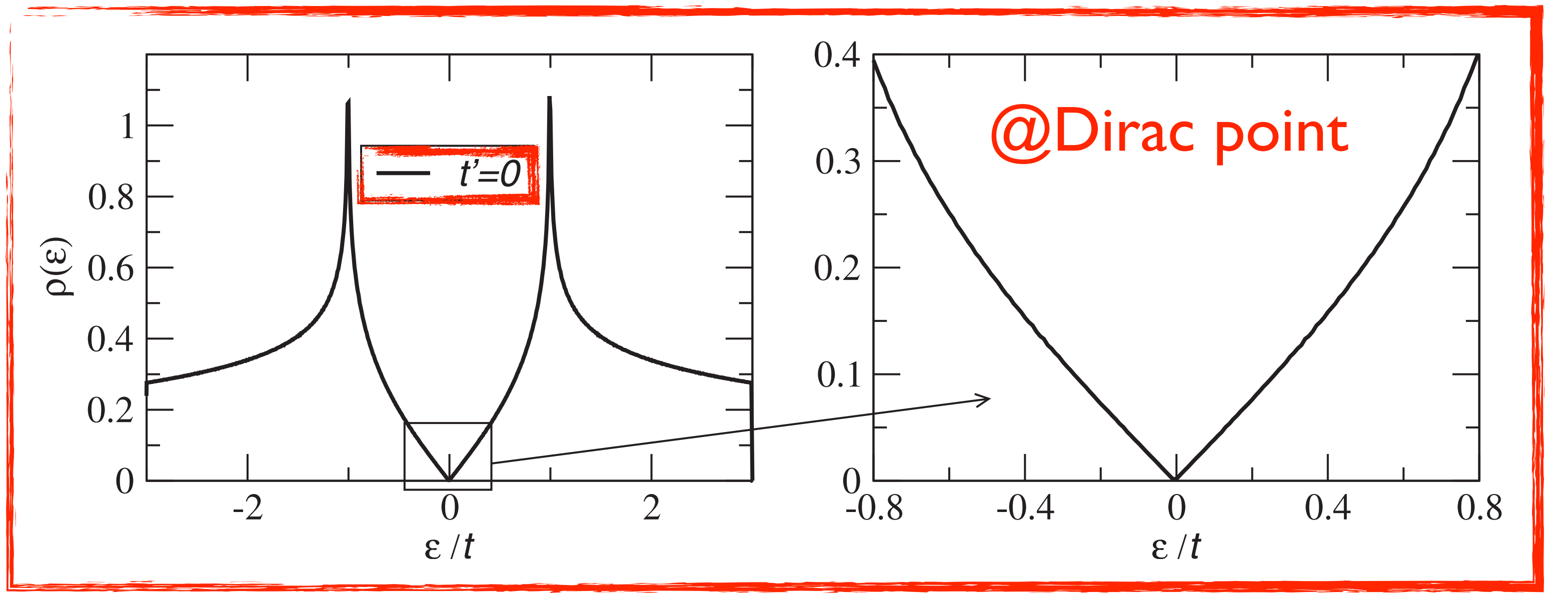


- Unprecedented phenomena in condensed matter:
  - *half integer quantum Hall effect*
  - *Klein paradox and suppression of backscattering*

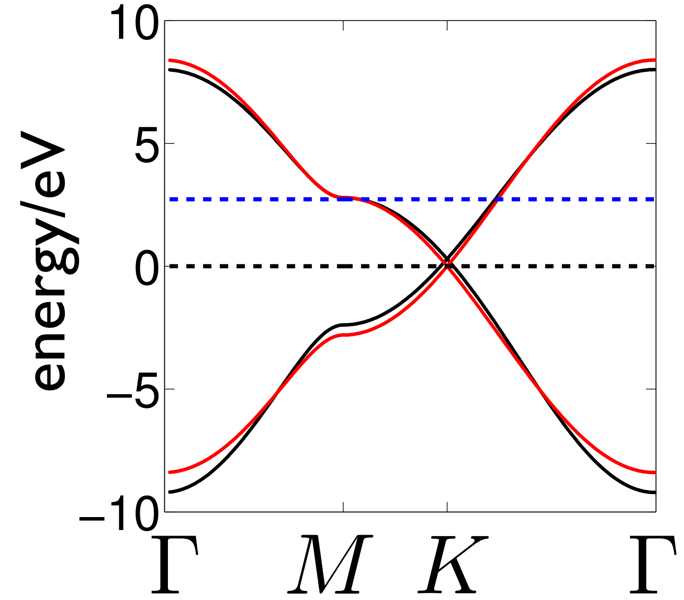
Castro Neto et al, Rev. Mod. Phys. **81**, 109 (2009)

Density of states

- Density of states: $\rho(\epsilon)$



energy dispersion



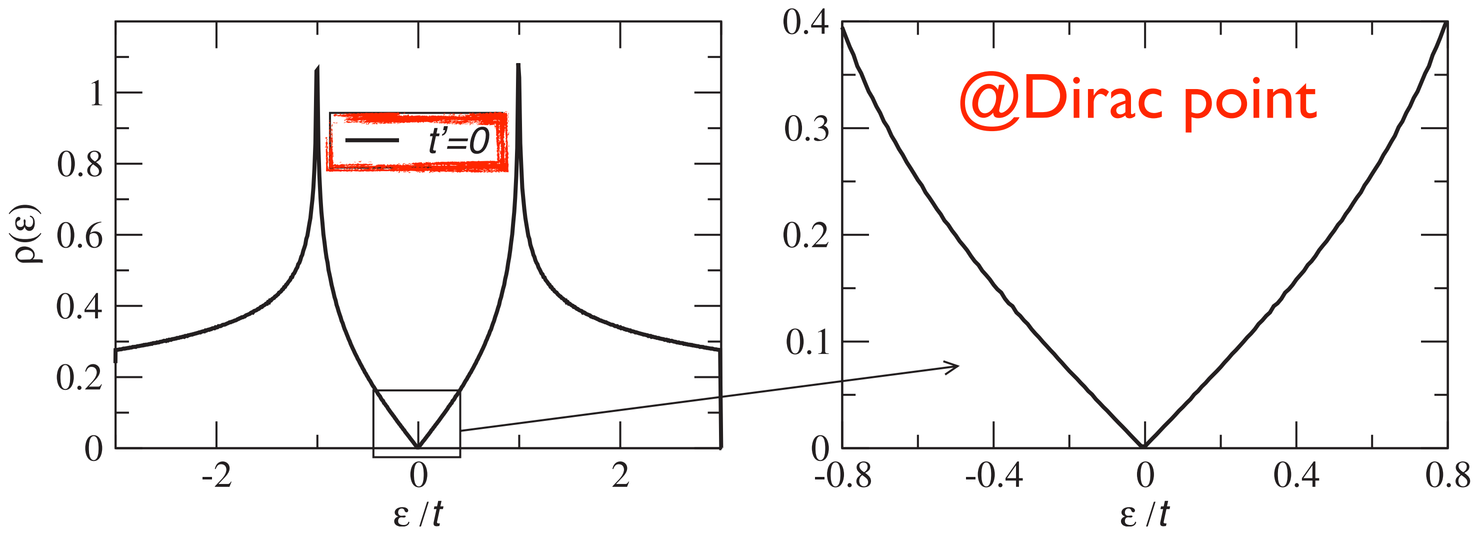
Kiesel et al, Phys. Rev. B **86**, 020507 (2012)

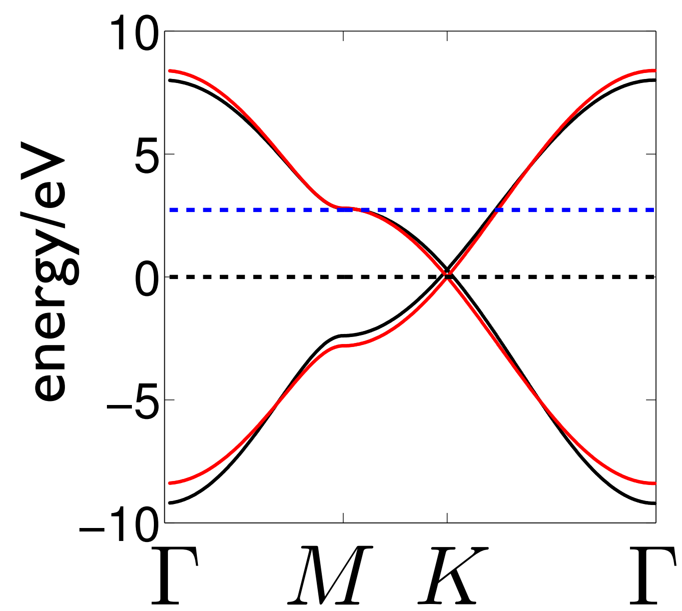
- close to Dirac point: $\rho(\epsilon) \propto |\epsilon|$

- van-Hove singularities @ finite doping → logarithmic divergence of $\rho(\epsilon)$

Density of states

- Density of states: $\rho(\epsilon)$





Kiesel et al, Phys. Rev. B **86**, 020507 (2012)

- close to Dirac point: $\rho(\epsilon) \propto |\epsilon|$
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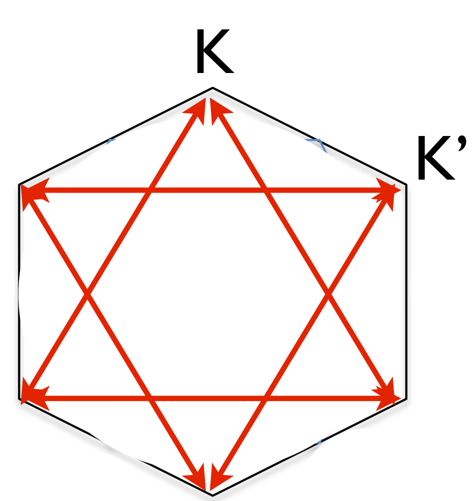
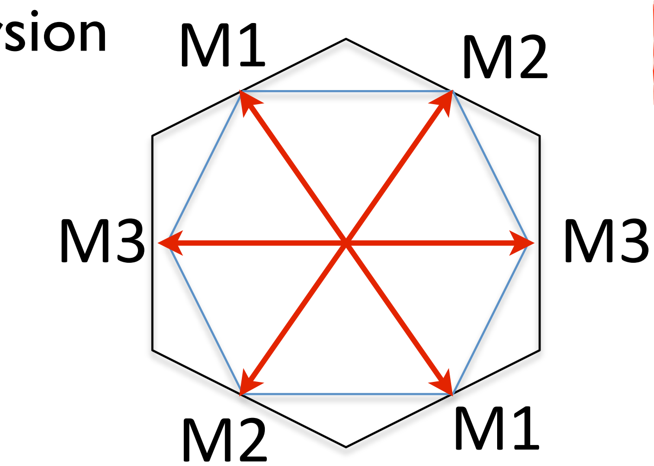
- **Graphene @ neutrality point:**
  - Dirac fermions
  - nesting
  - vanishing DOS



- **Graphene @ van-Hove singularity:**
  - saddle-point dispersion
  - nesting
  - diverging DOS



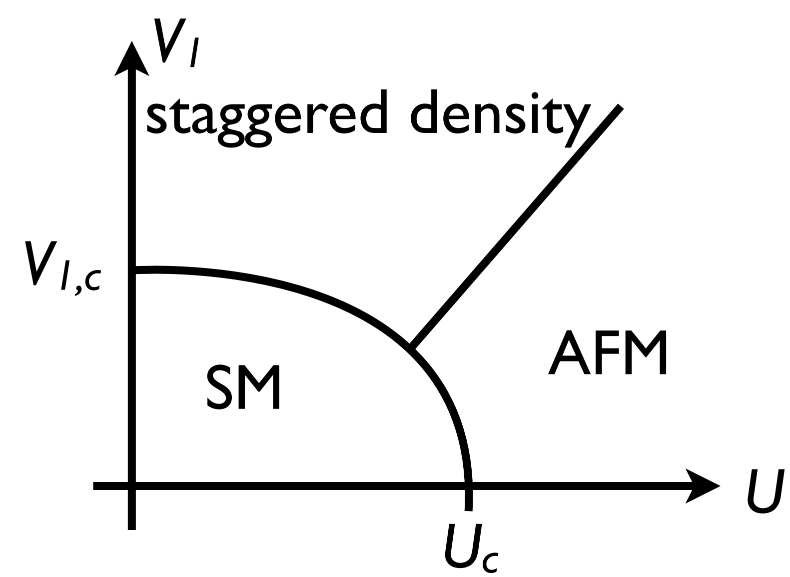
Interactions & phase transitions

$$H_{\rm int} = U\sum_i n_{i,\uparrow}n_{i,\downarrow} + V_1 \sum_{\langle i,j\rangle,\sigma,\sigma'} n_{i,\sigma}n_{j,\sigma'} + V_2 \sum_{\langle\langle i,j\rangle\rangle,\sigma,\sigma'} n_{i,\sigma}n_{j,\sigma'} + V_3 \sum_{\langle\langle\langle i,j\rangle\rangle\rangle,\sigma,\sigma'} n_{i,\sigma}n_{j,\sigma'}$$

	Graphene		Graphite	
	Bare	cRPA	Bare	cRPA
$U_{00}^{A\,\mathrm{or}\,B}$ (eV)	17.0	9.3	17.5, 17.7	8.0, 8.1
U_{01} (eV)	8.5	5.5	8.6	3.9
$U_{02}^{A\,\mathrm{or}\,B}$ (eV)	5.4	4.1	5.4, 5.4	2.4, 2.4
U_{03} (eV)	4.7	3.6	4.7	1.9

Wehling et al, Phys. Rev. Lett. **106**, 236805 (2011)

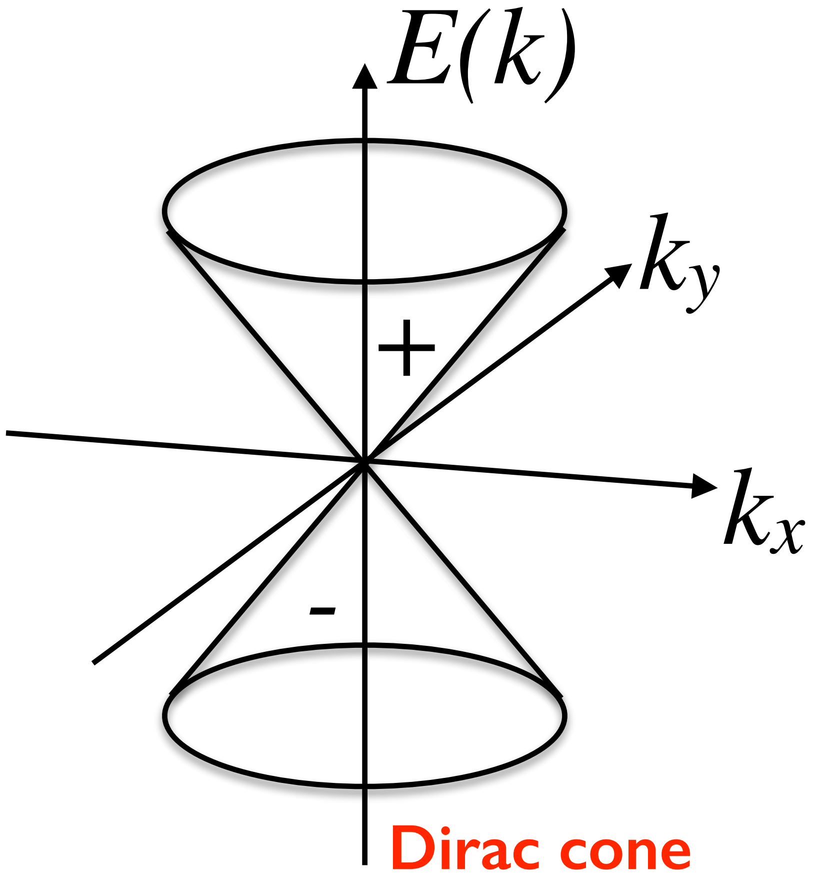
- **Undoped graphene → interactions can induce phase transitions:**
  - ✳ Dirac fermions have vanishing DOS at Fermi level
  - ✳ Stoner-type criterion → critical interaction strength required
  - ✳ Experimental data: Graphene below critical strength



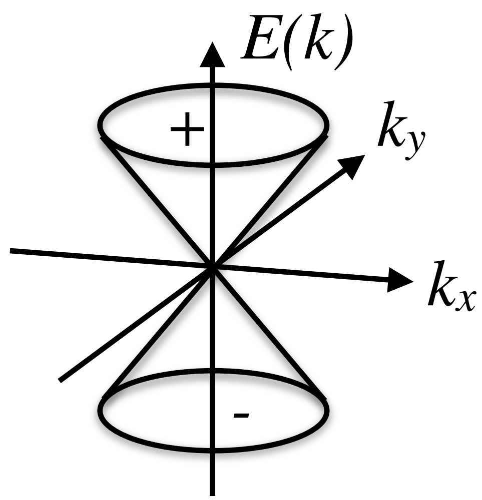
- **Graphene @ VHS → interactions can induce phase transitions:**
  - ✳ nesting: ph-channel diverges @ low T
  - ✳ also: pp-channel diverges @ low T

➡ competing orders

(F)RG aspects of **undoped** graphene



Symmetries & Fierz transformations



- Minimal description of i.a. electrons in graphene @ low energies?
- Symmetries of continuum interacting theory?
- What kinds of order expected? Nature of phase transitions?

- Start with linearized non-interacting Lagrangian for Dirac electrons: $L_0 = \bar{\Psi}(\vec{x},\tau)\gamma_\mu \partial_\mu \Psi(\vec{x},\tau)$
- Interactions (quartic, local,… and spinless): $L_{int} = (\Psi^\dagger(\vec{x},\tau) M_1 \Psi(\vec{x},\tau))(\Psi^\dagger(\vec{x},\tau) M_2 \Psi(\vec{x},\tau))$

4d hermitian matrices

Herbut, Phys. Rev. Lett. **97**, 146401 (2006)

Herbut et al., Phys. Rev. B **79**, 085116 (2009)

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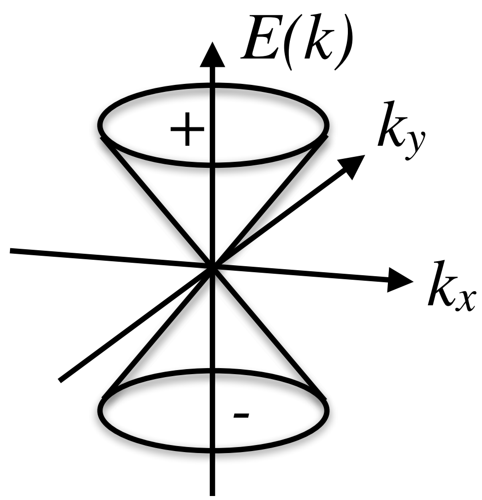

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  4d hermitian matrices

➡ **136 independent couplings in spinless case!**

- Honeycomb lattice symmetries help to reduce to 15 independent couplings

- Further reduction by Fierz identities!

➡ 6 independent couplings in spinless case!

Herbut, Phys. Rev. Lett. **97**, 146401 (2006)

Herbut et al., Phys. Rev. B **79**, 085116 (2009)

Symmetries, Fierz transformations & order parameters

- Reduction of independent couplings can be pushed further
  - near quantum critical point additional symmetries from non-interacting theory restored…
  - minimal low-energy description of i.a. spinless honeycomb electrons:

Symmetries:

- Reflection
- Translation
- Time-reversal
- Rotations
- Lorentz
- Chiral

$$L = L_0 + g_{D2}(\bar{\Psi}\gamma_{35}\Psi)^2 + g_{C1}(\bar{\Psi}\Psi)^2$$

- order parameter: QAH
- order parameter: CDW

Herbut, Phys. Rev. Lett. **97**, 146401 (2006)

Herbut et al., Phys. Rev. B **79**, 085116 (2009)

FRG phase transitions & critical behavior

- Situation with spin works similarly - e.g. obtain AF-SDW order and CDW order
- Introduce order parameter fields via Hubbard-Stratonovich transformation

order parameter field Z_2 or SO(3)

$$\Gamma_k = \int \mathrm{d}^D x \Big[Z_{\Psi,k} \bar{\Psi} \left(\mathbb{1}_2 \otimes \gamma_\mu \right) \partial_\mu \Psi - \frac{1}{2} Z_{\phi,k} \phi_a \partial_\mu^2 \phi_a + U_k(\rho) + \bar{g}_k \phi_a \bar{\Psi} \left(\sigma_a \otimes \mathbb{1}_4 \right) \Psi \Big],$$

Janssen & Herbut, Phys. Rev. B **89**, 205403 (2014)

Janssen & Gies, Phys. Rev. D **86**,105007 (2012)

Mesterhazy et al., Phys. Rev. B **86**, 245431 (2012)

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& have fun:

$$\partial_t \Gamma_k = \frac{1}{2} \mathrm{STr} \left[\partial_t \mathrm{R}_k \left(\Gamma_k^{(2)} + \mathrm{R}_k \right)^{-1} \right]$$

▸ quantify critical behaviour at quantum phase transition (Z_2):

	$1/\nu$	η_ϕ	η_Ψ
FRG [LPA', $\mathcal{O}(\tilde{\rho}^6)$, $\mathrm{R}_k^{\mathrm{lin}}$]	0.982	0.760	0.032
FRG [LPA', $\mathcal{O}(\tilde{\rho}^6)$, $\mathrm{R}_k^{\mathrm{sc}}$]	0.978	0.767	0.033
FRG [LPA', full $u(\tilde{\rho})$, $\mathrm{R}_k^{\mathrm{lin}}$] [21]	0.982	0.756	0.032
$1/N_\mathrm{f}$-expansion (2nd/3rd order) [34,35]	0.962*	0.776	0.044
$(2+\epsilon)$-expansion (3rd order) [28]	0.764	0.602	0.081
$(4-\epsilon)$-expansion (2nd order) [13,33]	1.055	0.695	0.065
Polynomial interpolation $P_{2,2}$	0.995	0.753	0.034
Polynomial interpolation $P_{3,2}$	0.949	0.716	0.041
Monte-Carlo simulations [33†]	1.00(4)	0.754(8)	–

▸ Graphene: AFM-Mott transition

▸ "chiral Heisenberg universality class"

➡ talk by L. Janssen

Janssen & Herbut, Phys. Rev. B **89**, 205403 (2014)

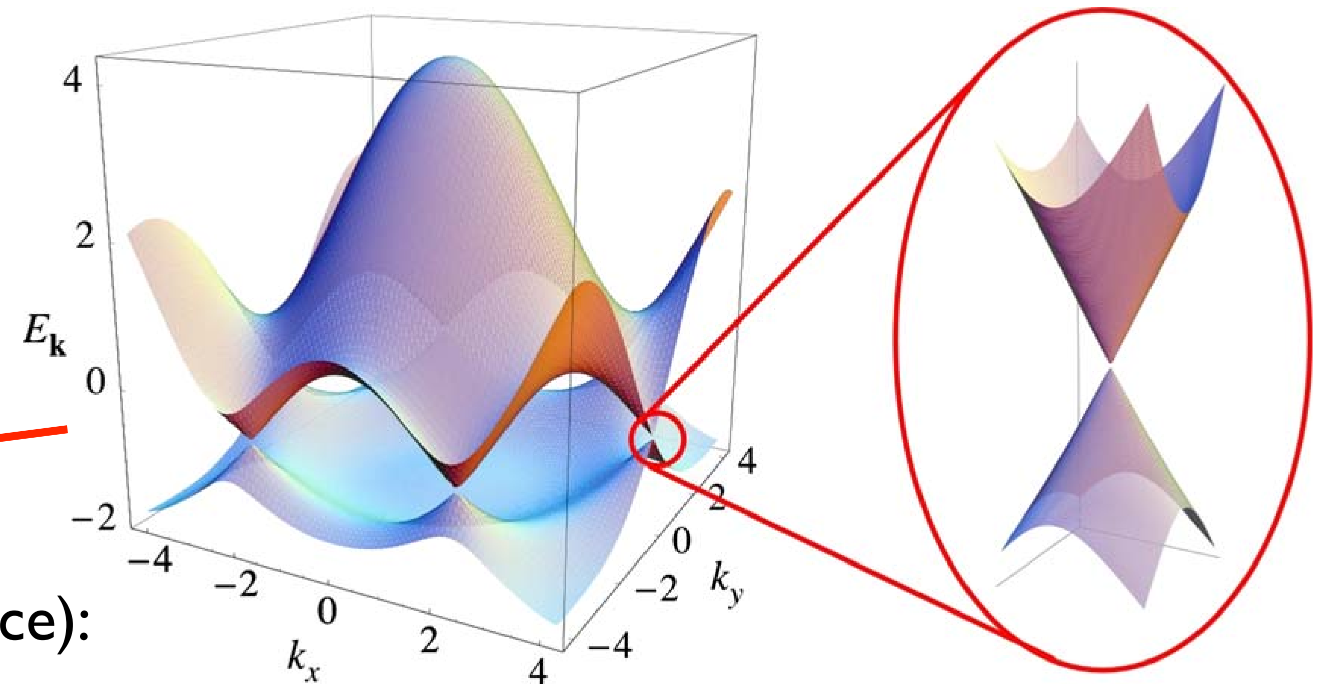
Janssen & Gies, Phys. Rev. D **86**,105007 (2012)

Mesterhazy et al., Phys. Rev. B **86**, 245431 (2012)

N-Patch FRG scheme

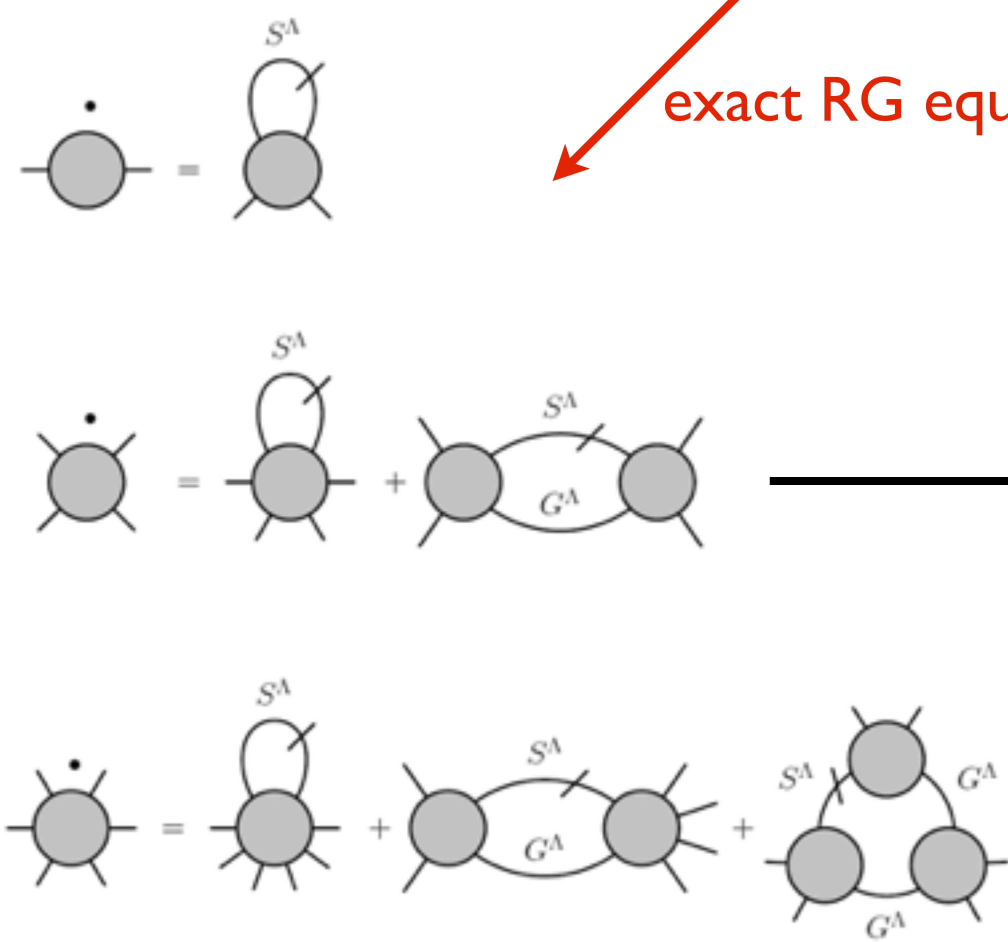
- Take into account full band structure
- Modified bare propagator with IR cutoff:

$$G_0^\Lambda(k_0, \mathbf{k}) = \frac{\theta^\Lambda(\mathbf{k})}{ik_0 - \xi_\mathbf{k}}$$



- Vertex expansion (with momentum dependence):

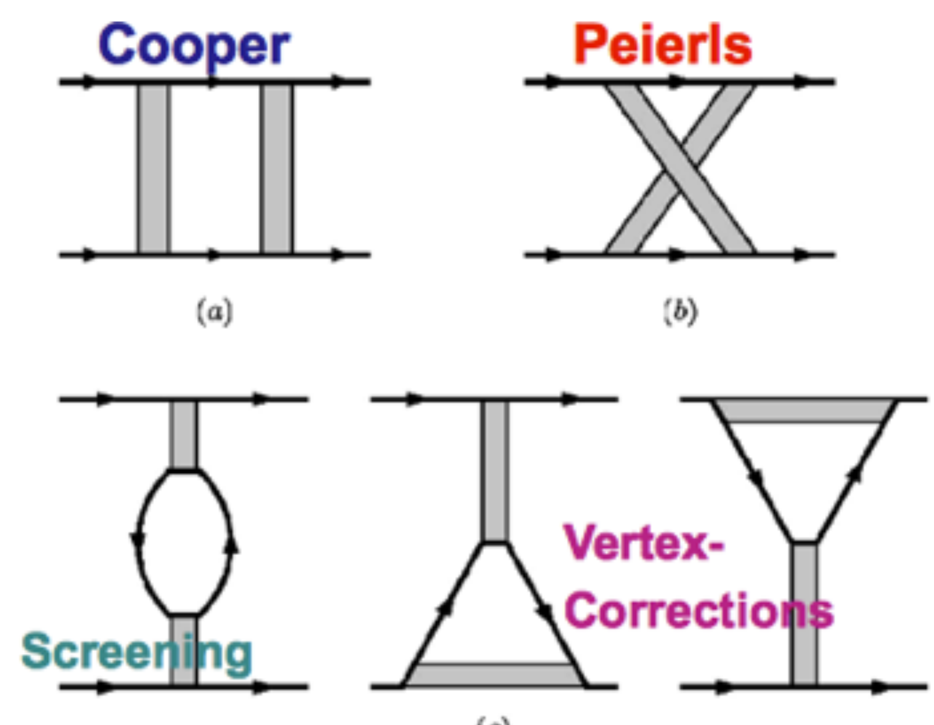
exact RG equation



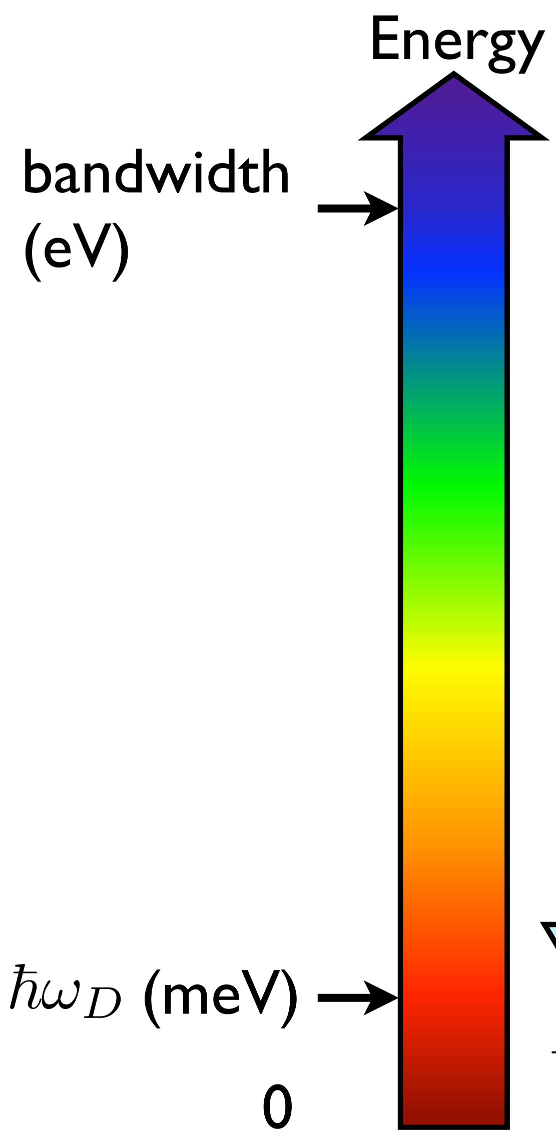
...

Salmhofer & Honerkamp, Prog. Theor. Phys. **105** (2001)

Metzner et al., Rev. Mod. Phys. **84,** 299 (2012)

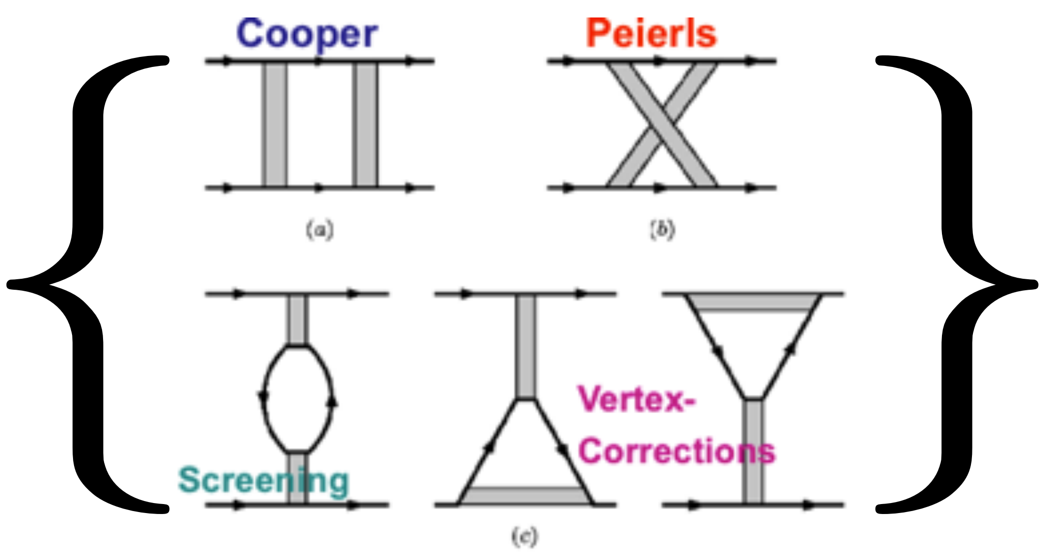
- Neglect 6-point and higher vertices
- No self-energy feedback
- 

N-Patch FRG scheme



$$H_{\text{bare}} = U \sum_i n_{i,\uparrow} n_{i,\downarrow} + V_1 \sum_{\langle i,j\rangle,\sigma,\sigma'} n_{i,\sigma} n_{j,\sigma'} + \ldots$$

FRG:

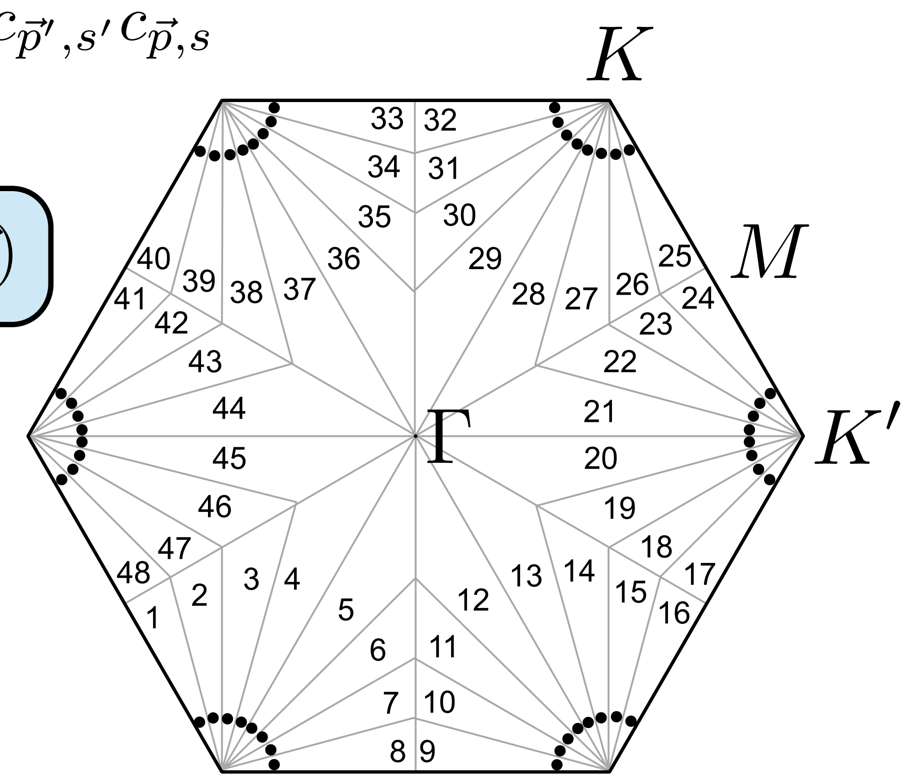


generate structure in low-energy interaction

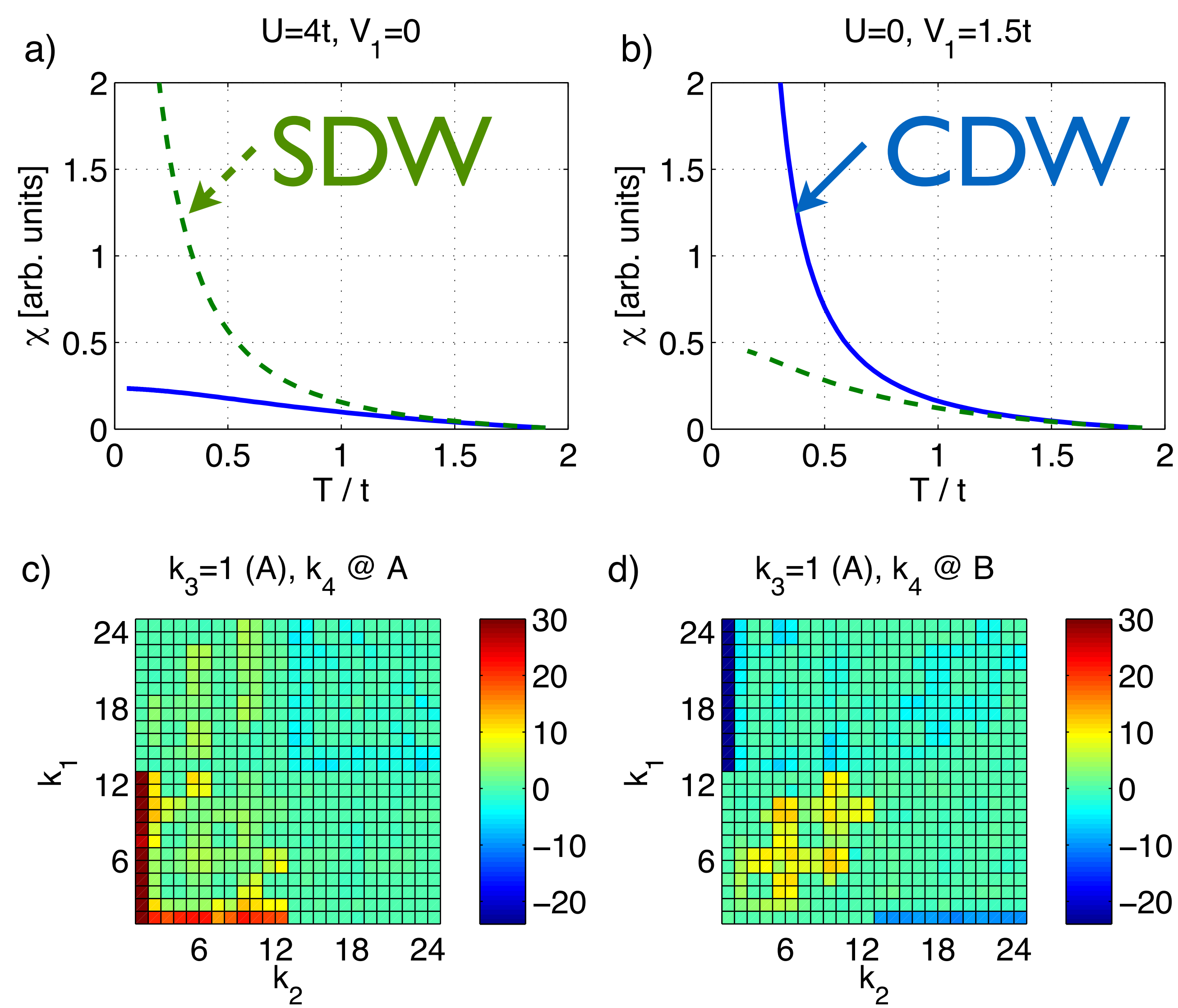
$$H_{\text{eff}} = \frac{1}{2} \sum_{\vec{p},\vec{p}',\vec{q},s,s'} V(\vec{p},\vec{p}',\vec{p}+\vec{q}) c^\dagger_{\vec{p}+\vec{q},s} c^\dagger_{\vec{p}'-\vec{q},s'} c_{\vec{p}',s'} c_{\vec{p},s}$$

- low-energy effective action & momentum structure $V(\vec{p},\vec{p}',\vec{p}+\vec{q})$

- Wavevector: discretized by **patching of Brillouin zone**
- Interaction constant within one patch



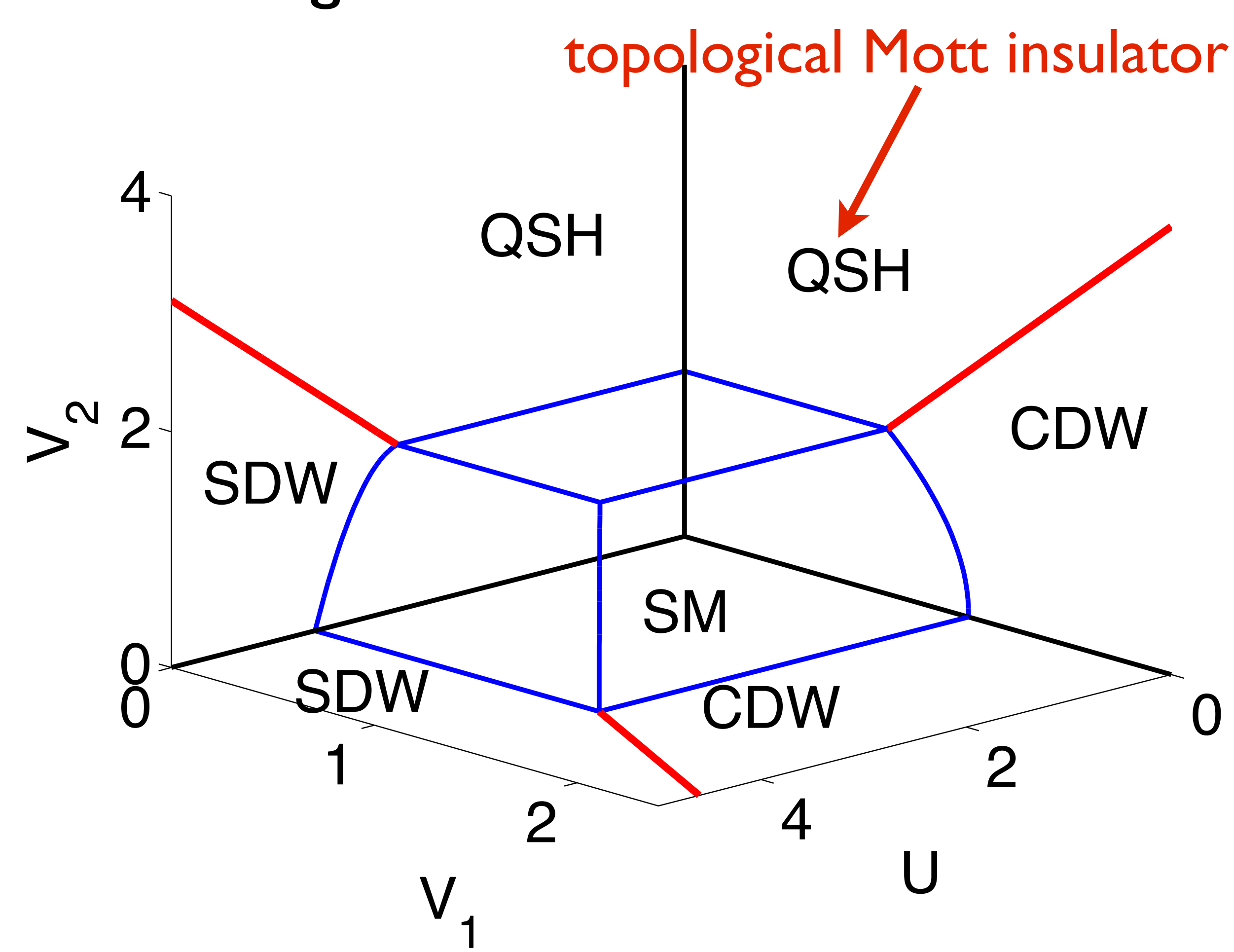
Density waves on the honeycomb lattice



$$H_{\text{int}} = U \sum_i n_{i,\uparrow} n_{i,\downarrow} + V_1 \sum_{\langle i,j \rangle,\sigma,\sigma'} n_{i,\sigma} n_{j,\sigma'} + V_2 \sum_{\langle\langle i,j \rangle\rangle,\sigma,\sigma'} n_{i,\sigma} n_{j,\sigma'}$$

$$\sim \sum_{\vec{q}} J_{\vec{q}}^{b,b'} \vec{S}_{\vec{q}}^{b} \cdot \vec{S}_{-\vec{q}}^{b'}$$

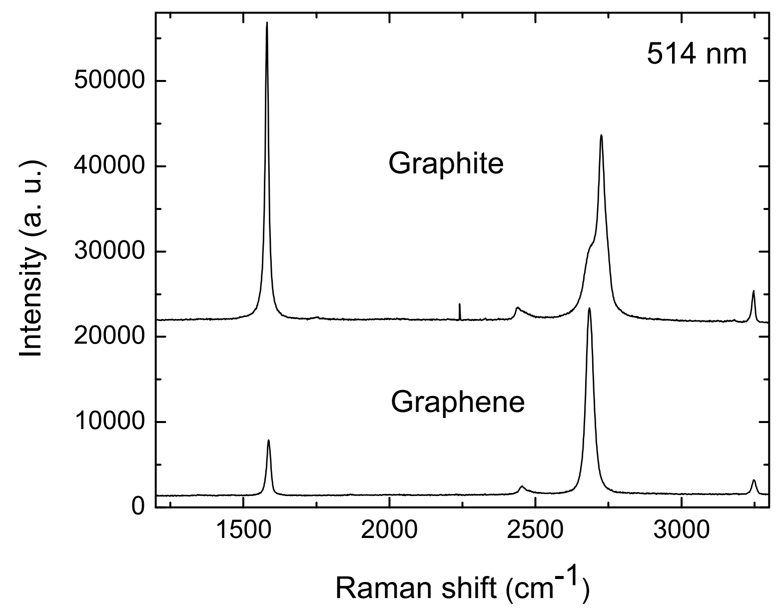
- **Phase diagram:**



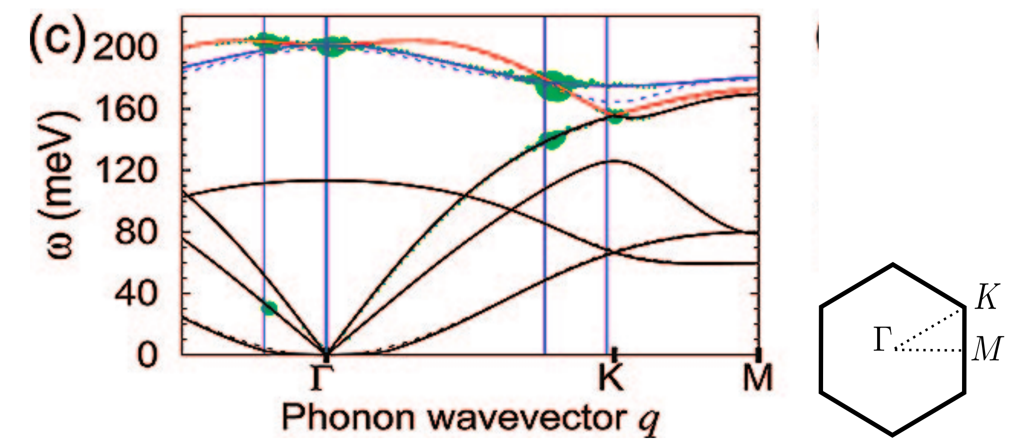
Honerkamp, Phys. Rev. Lett. 100, 146404 (2008)
Raghu et al., Phys. Rev. Lett. 100, 156401 (2008)

Phonon-induced electron-electron interactions

- Lattice vibrations (Raman spectroscopy)

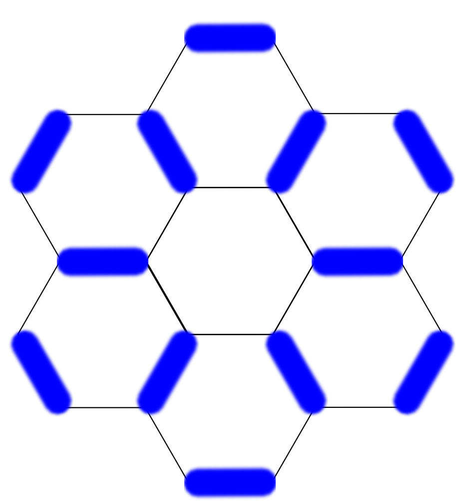


A. C. Ferrari *et al.* PRL **97** (2006)

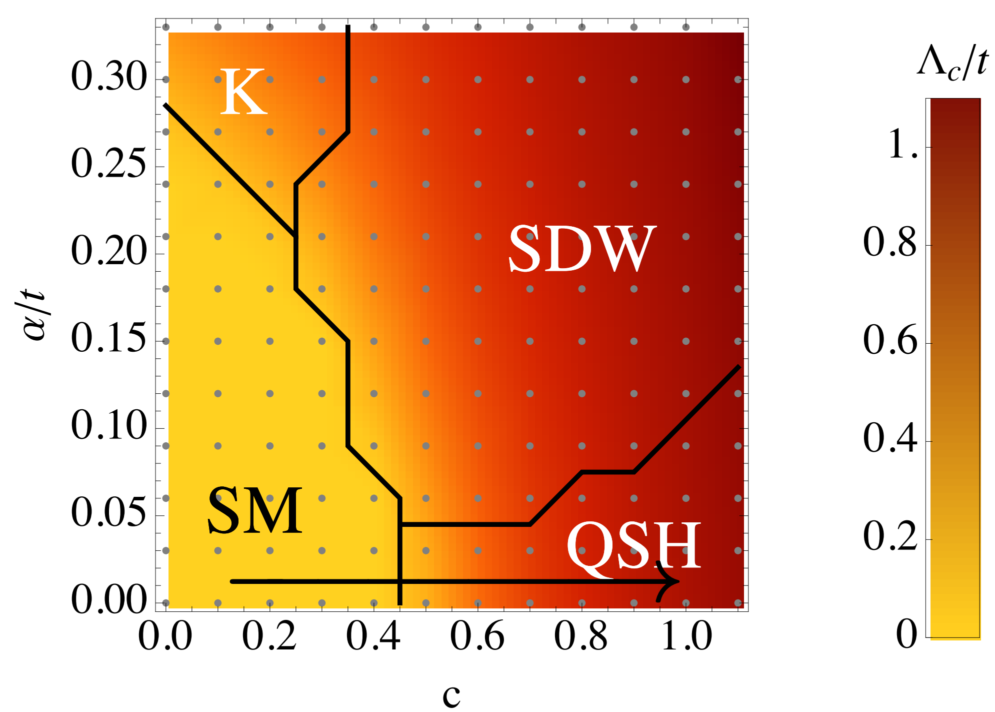


C. Park *et al.* NL **8** (2008)

- Modified hopping $t \to t + dt$
  → EPC coupling induces Kekule instability:



- Phase diagram with short-ranged Coulomb i.a.:

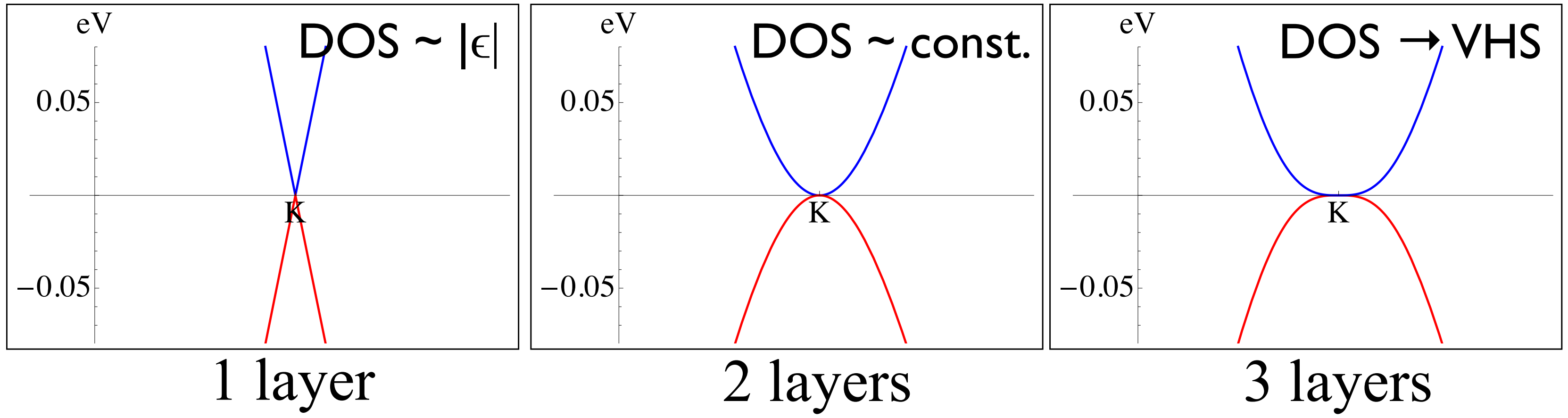


$\{U/t, V_1/t, V_2/t\} \approx \{3.3, 2.0, 1.5\}$
$\to c\,\{U/t, V_1/t, V_2/t\}$

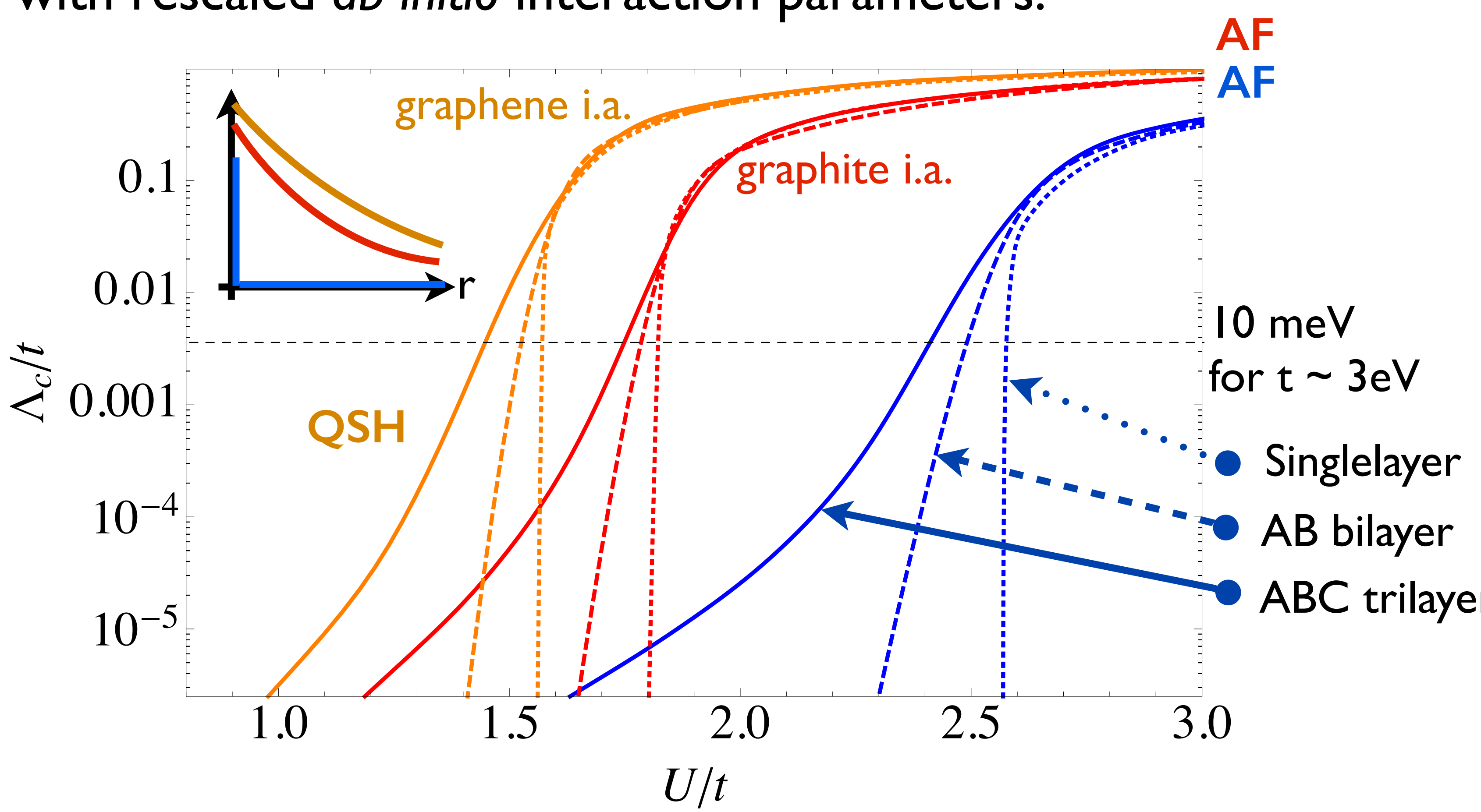
Classen, MMS, Honerkamp, Phys. Rev. B **90**, 035122 (2014)

➡ talk by L. Classen

Critical scales of honeycomb stacks



- Critical scales with rescaled *ab initio* interaction parameters:

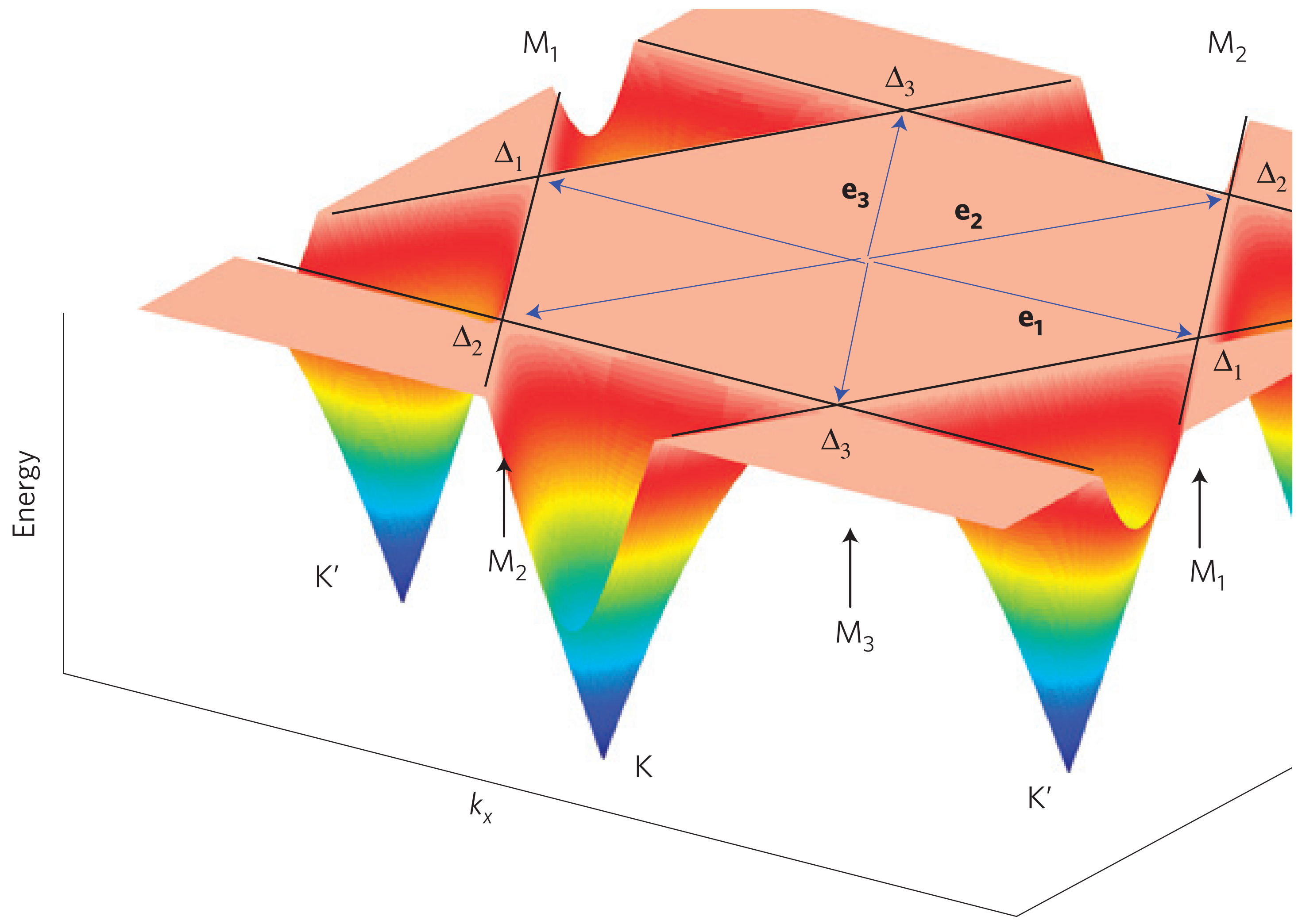


- ABC trilayer most prone to instabilities, critical scale drops quickly when $U < U_{c,\text{Singlelayer}}$
- *Ab initio* parameters put system close to QSH/AFM phase boundary

MMS, Uebelacker, Honerkamp, Phys. Rev. B **85**, 235408 (2012)

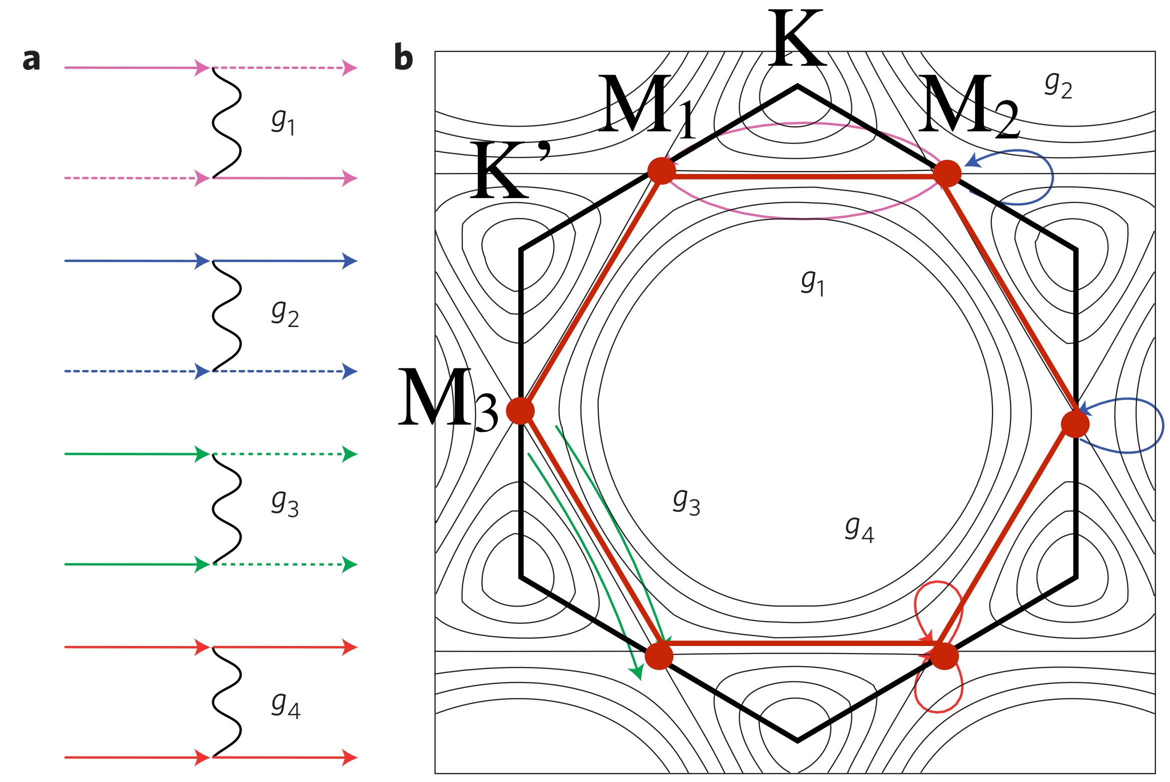
MMS, Uebelacker, DDScherer, Honerkamp, Phys. Rev. B **86**, 155415 (2012)

(F)RG aspects of graphene @ VHS



RG for graphene @VHS - **g-ology**

$$\mathcal{L} = \sum_{\alpha=1}^{3} \psi_\alpha^\dagger (\partial_\tau - \epsilon_{\mathbf{k}} + \mu)\psi_\alpha - \frac{1}{2} g_4 \psi_\alpha^\dagger \psi_\alpha^\dagger \psi_\alpha \psi_\alpha$$
$$- \sum_{\alpha \neq \beta} \frac{1}{2} \left[g_1 \psi_\alpha^\dagger \psi_\beta^\dagger \psi_\alpha \psi_\beta + g_2 \psi_\alpha^\dagger \psi_\beta^\dagger \psi_\beta \psi_\alpha + g_3 \psi_\alpha^\dagger \psi_\alpha^\dagger \psi_\beta \psi_\beta \right]$$



- RG equations:

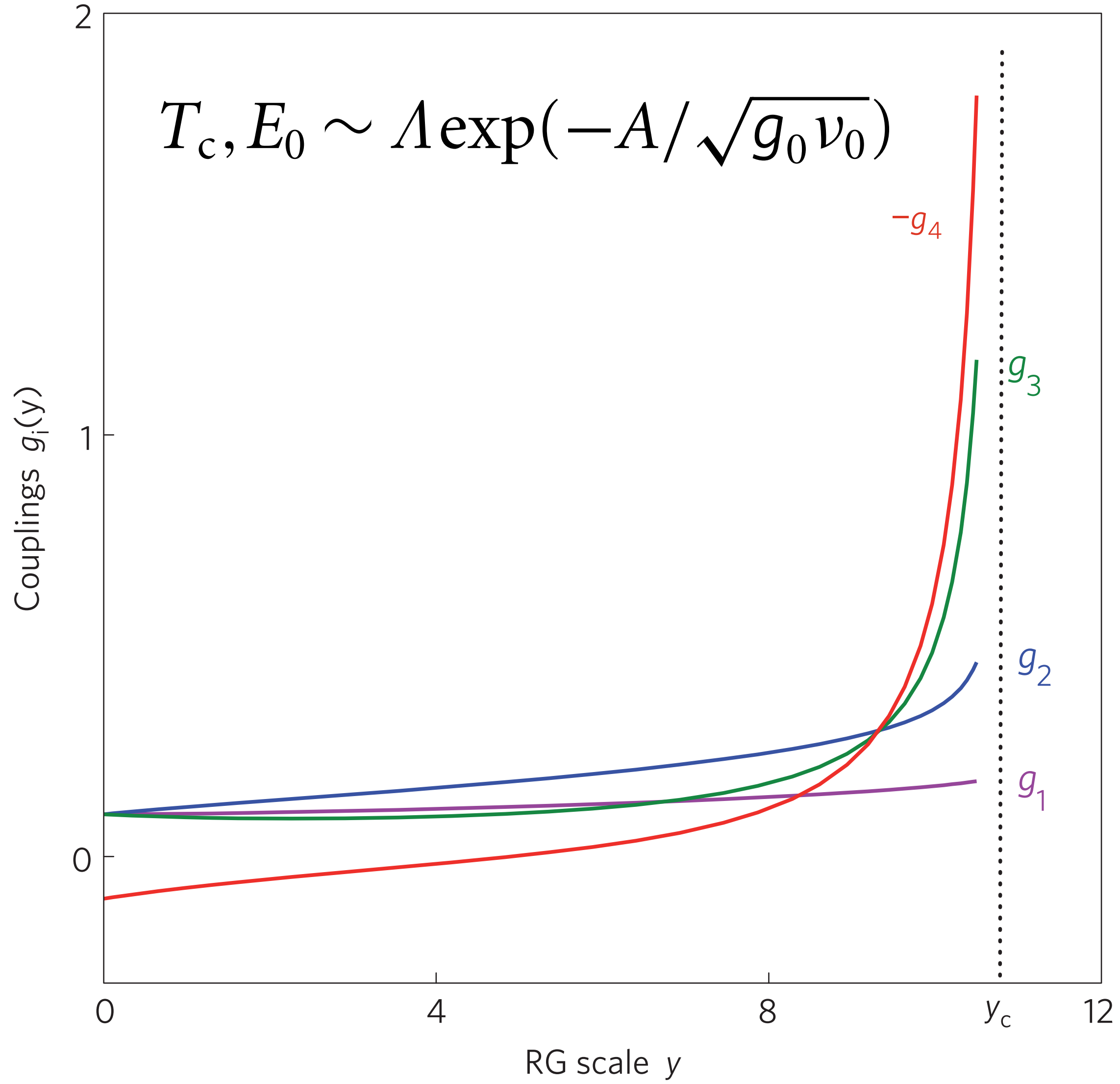
$$\frac{dg_1}{dy} = 2d_1 g_1 (g_2 - g_1), \quad \frac{dg_2}{dy} = d_1 (g_2^2 + g_3^2)$$
$$\frac{dg_3}{dy} = -(n-2) g_3^2 - 2 g_3 g_4 + 2 d_1 g_3 (2 g_2 - g_1),$$
$$\frac{dg_4}{dy} = -(n-1) g_3^2 - g_4^2$$

- reproduce two-patch RG for n=2
- Graphene at VHS needs n=3

Nandkishore, Levitov, Chubukov, Nature Physics **8**, 158 (2012)

Furukawa, Rice, Salmhofer, Phys. Rev. Lett. **81**, 3195–3198 (1998)

RG for graphene @VHS - g-ology



- Susceptiblities (introduce test vertices)

$$\delta \mathcal{L} = \sum_{\alpha=1}^{3} \tilde{\Delta}_\alpha \psi^\dagger_{\alpha,\uparrow} \psi^\dagger_{\alpha,\downarrow} + \tilde{\Delta}^*_\alpha \psi_{\alpha,\uparrow} \psi_{\alpha,\downarrow}$$

- d-wave SC susceptibility

$$\chi_{\mathrm{dSC}}(y) \sim (y_c - y)^{-1.5}$$

- AF-SDW susceptibility @perfect nesting

$$\chi_{\mathrm{SDW}}(y) \sim (y_c - y)^{-1}$$

- Close competition between SDW and dSC
- dSC is leading instability for all values of nesting

  ➡ in contrast to square lattice (SDW@perfect nesting)

Nandkishore, Levitov, Chubukov, Nature Physics **8**, 158 (2012)

FRG for graphene @VHS - **N-Patch FRG**

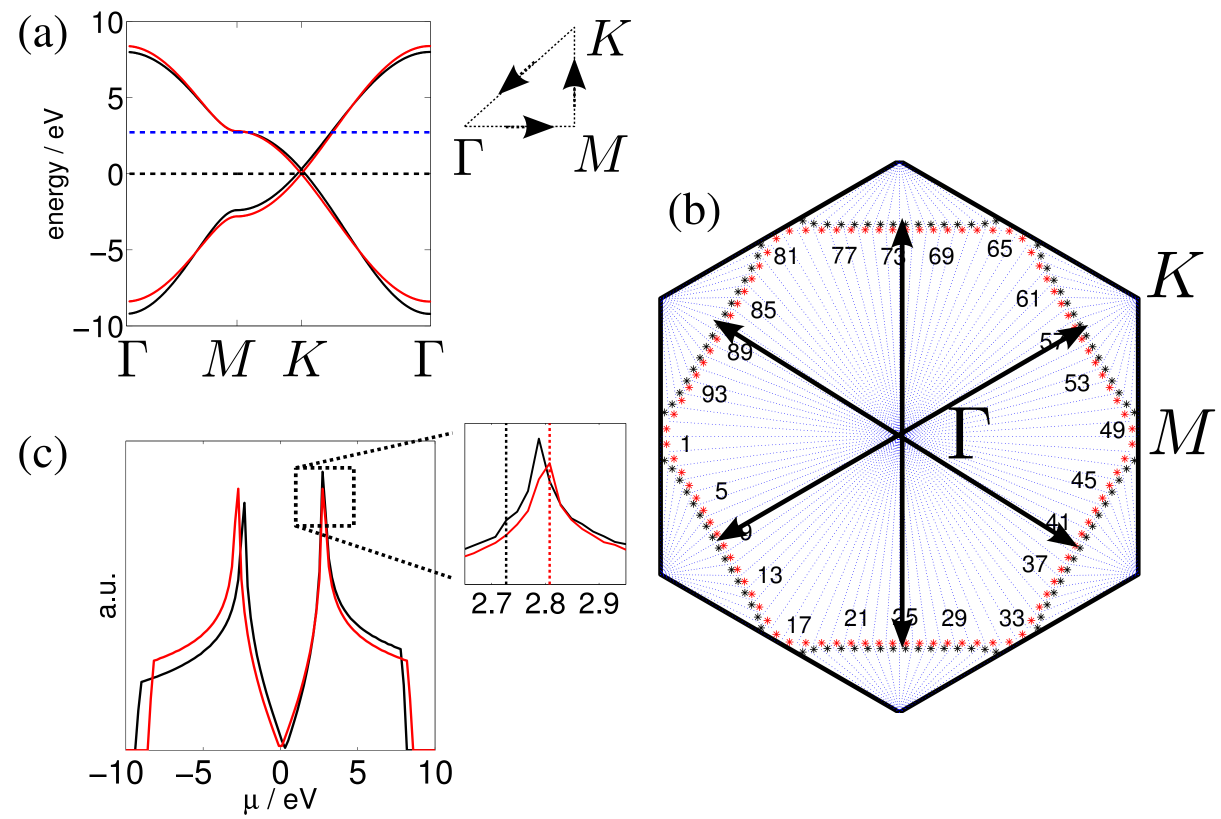
- Full band structure & realistic model parameters:

$$H_0 = \Big[t_1 \sum_{\langle i,j\rangle} \sum_{\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + t_2 \sum_{\langle\langle i,j\rangle\rangle} \sum_{\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + t_3 \sum_{\langle\langle\langle i,j\rangle\rangle\rangle} \sum_{\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \text{h.c.}\Big] - \mu n,$$

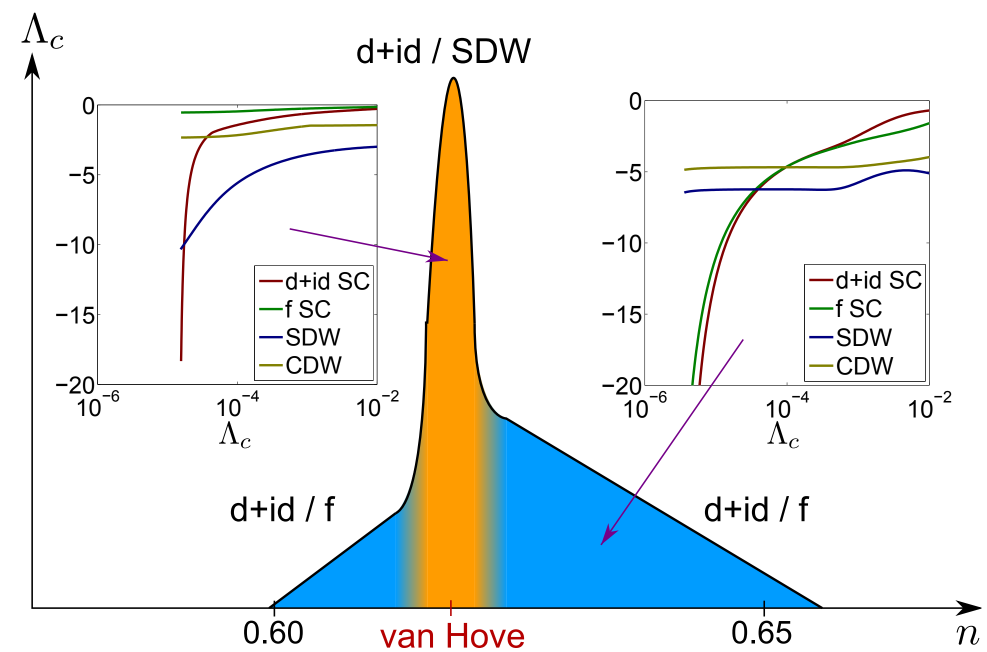
- Interaction terms:

	Graphene		Graphite	
	Bare	cRPA	Bare	cRPA
$U_{00}^{A \text{ or } B}$ (eV)	17.0	9.3	17.5, 17.7	8.0, 8.1
U_{01} (eV)	8.5	5.5	8.6	3.9
$U_{02}^{A \text{ or } B}$ (eV)	5.4	4.1	5.4, 5.4	2.4, 2.4
U_{03} (eV)	4.7	3.6	4.7	1.9

Wehling et al, Phys. Rev. Lett. **106**, 236805 (2011)



- longer-range hoppings decrease degree of nesting
- dSC wins
- with realistic parameters: T_c ~ a few K



Kiesel, Platt, Hanke, Abanin, Thomale, Phys. Rev. B **86**, 020507 (2012)

Wang et al, Phys. Rev. B **85**, 035414 (2012)

Conclusions & Outlook

Graphene allows for beautiful/useful/complex/unprecedented/exotic theory!

- Phase transitions and criticality @Dirac point
  - precision estimates - dynamical bosonization, higher-derivative terms? multicriticality?
- Phase transitions and criticality @VHS - realization of chiral d-wave superconductor?
  - coupling to the lattice
  - self-energy effects
  - van Hove situation difficult to assess by other methods (finite-size, sign problems)
  - collective fluctuations, cf. Krahl, Friederich, Wetterich on Hubbard model
- Methods & related materials:
  - spin-SU(2) - extend scheme to include SOC ➡ **talks by D. Scherer & G. Schober**
  - multiorbital models ➡ **talk by C. Platt**