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Phase transitions, **quantum critical behavior** and emergent symmetries of **interacting Dirac materials**

—

Renormalization group approach(es)

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Outline

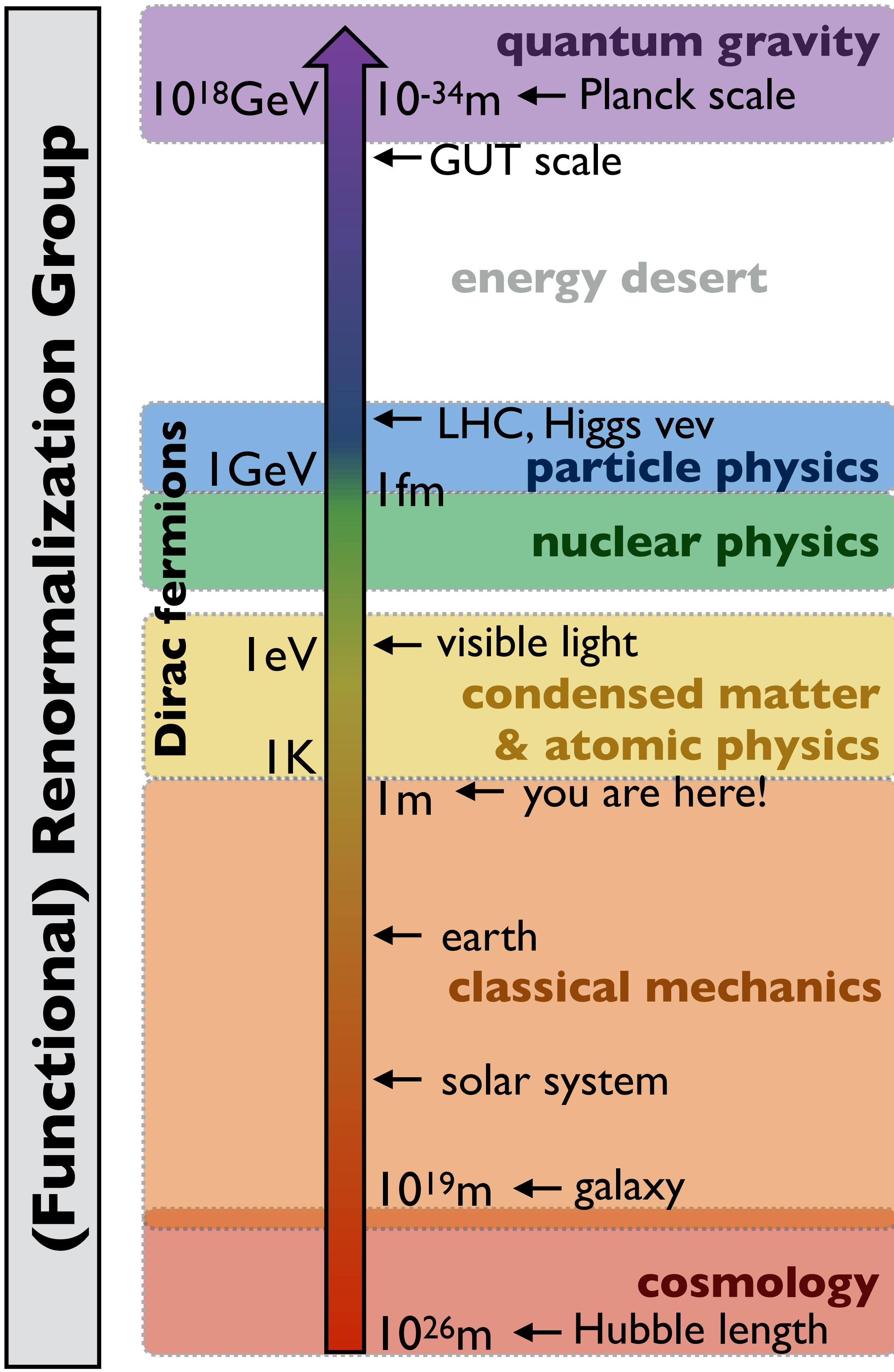
— Introduction —

(I) Many-body instabilities of honeycomb electrons from functional RG

(II) Dirac fermions and critical phenomena from perturbative RG

— Conclusion —

Physics of scales



fundamental particles in cond-mat:

- low-energy excitations

  ➡ can behave as Dirac/Weyl fermions:

$$H_D = c\boldsymbol{\sigma} \cdot \mathbf{p} + mc^2\sigma_z$$

- **universal properties:**

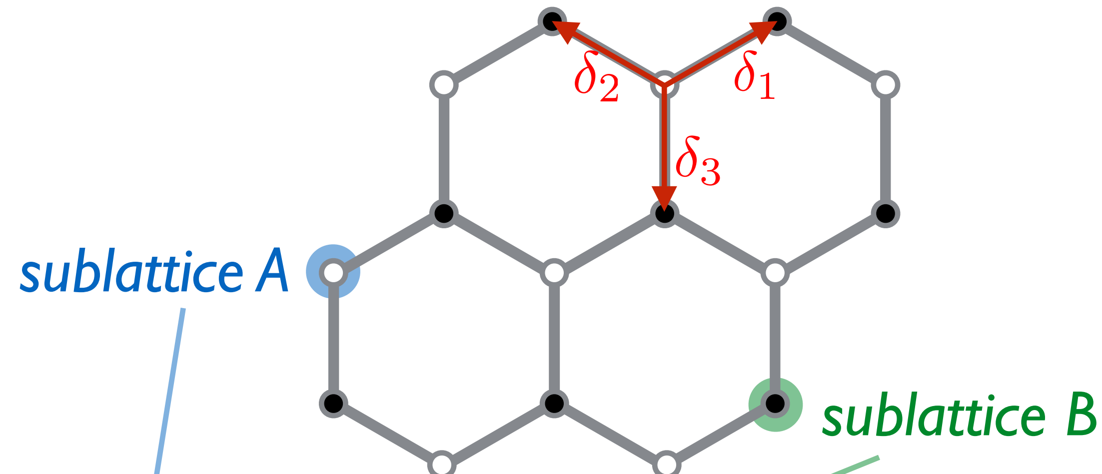
  DOS, specific heat, transport,

  thermodynamic properties, …

- **Dirac/Weyl fermions** emerge in:
  - *d-wave superconductors*
  - *graphene, Na_3Bi,…*
  - *topological insulators*

Electrons on the **honeycomb** lattice

- focus on **2D Dirac materials** with electron quasiparticles (graphene)
  - lattice in real space:

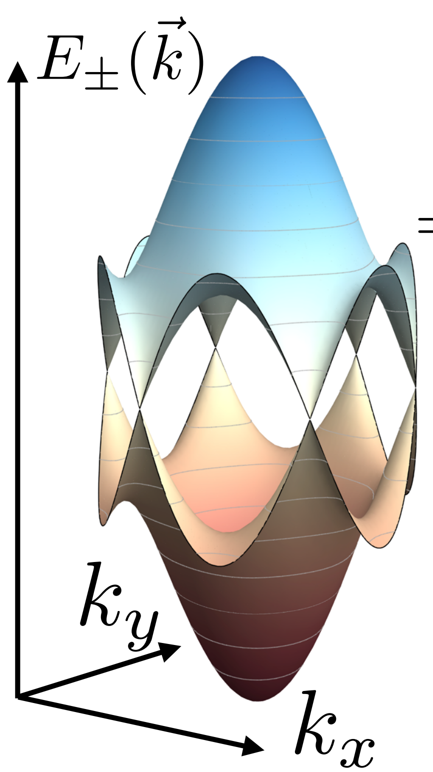


  - tight-binding Hamiltonian:

$$H_0 = -t \sum_{\sigma, \vec{R}, \vec{\delta}_i} \left[u^\dagger_\sigma(\vec{R}) v_\sigma(\vec{R} + \vec{\delta}_i) + \text{h.c.} \right]$$

$$= \sum_{\sigma, \vec{R}, \vec{\delta}_i} \left(u^\dagger_\sigma(\vec{R}), v^\dagger_\sigma(\vec{R} + \vec{\delta}_i) \right) \begin{pmatrix} 0 & -t \\ -t & 0 \end{pmatrix} \begin{pmatrix} u_\sigma(\vec{R}) \\ v_\sigma(\vec{R} + \vec{\delta}_i) \end{pmatrix}$$

$$= \sum_{\sigma, \vec{k}} \left(u^\dagger_\sigma(\vec{k}), v^\dagger_\sigma(\vec{k}) \right) \begin{pmatrix} 0 & -t\, d(\vec{k}) \\ -t\, d^*(\vec{k}) & 0 \end{pmatrix} \begin{pmatrix} u_\sigma(\vec{k}) \\ v_\sigma(\vec{k}) \end{pmatrix} \quad \text{where} \quad d(\vec{k}) = \sum_{\vec{\delta}_i} e^{i \vec{k} \cdot \vec{\delta}_i}$$



➡ energy dispersion from diagonalization: $E_\pm(\vec{k}) = \pm t \, |d(\vec{k})|$

  - two energy bands for each spin projection!

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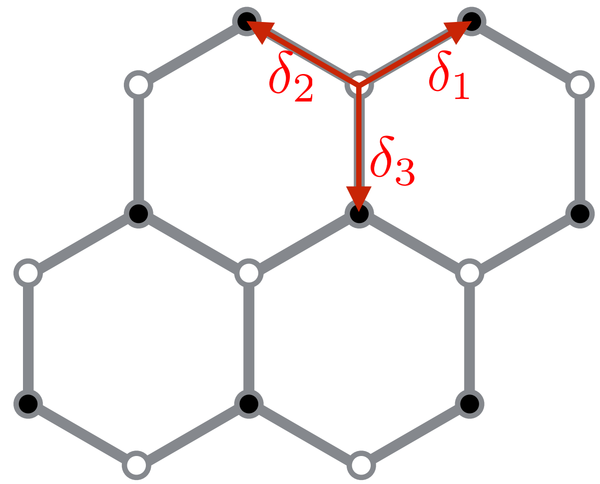
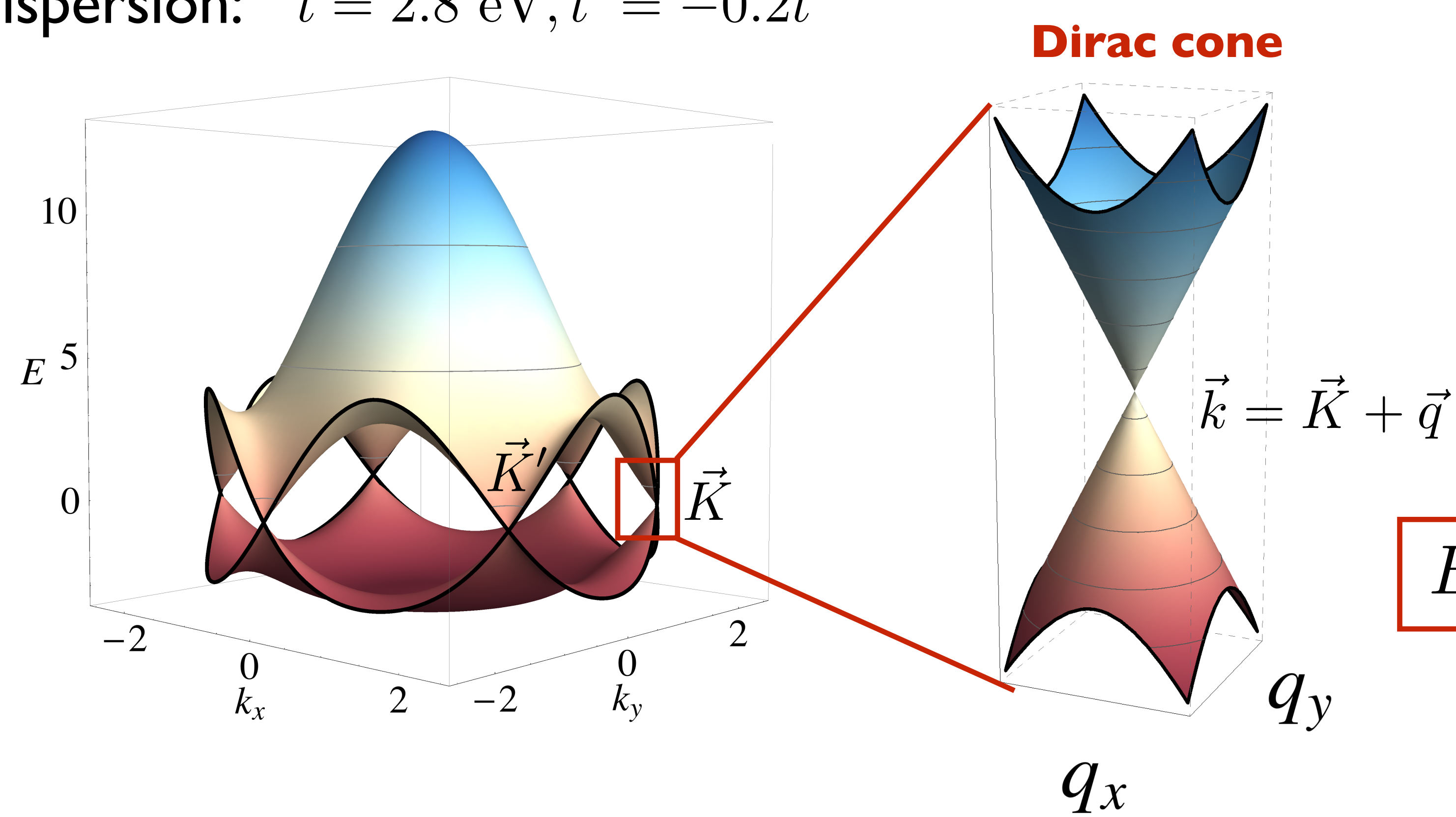


  - tight-binding Hamiltonian: $H_0 = -t \sum_{\vec{R},i} \left[u^\dagger(\vec{R}) v(\vec{R} + \vec{\delta}_i) + \text{h.c.} \right] + \ldots$
  - energy dispersion: $t = 2.8\ \text{eV}, t' = -0.2t$



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

  - no gap + vanishing density of states → **semimetallic** behavior

Electron-electron **interactions**

local interaction — *Coulomb tail*

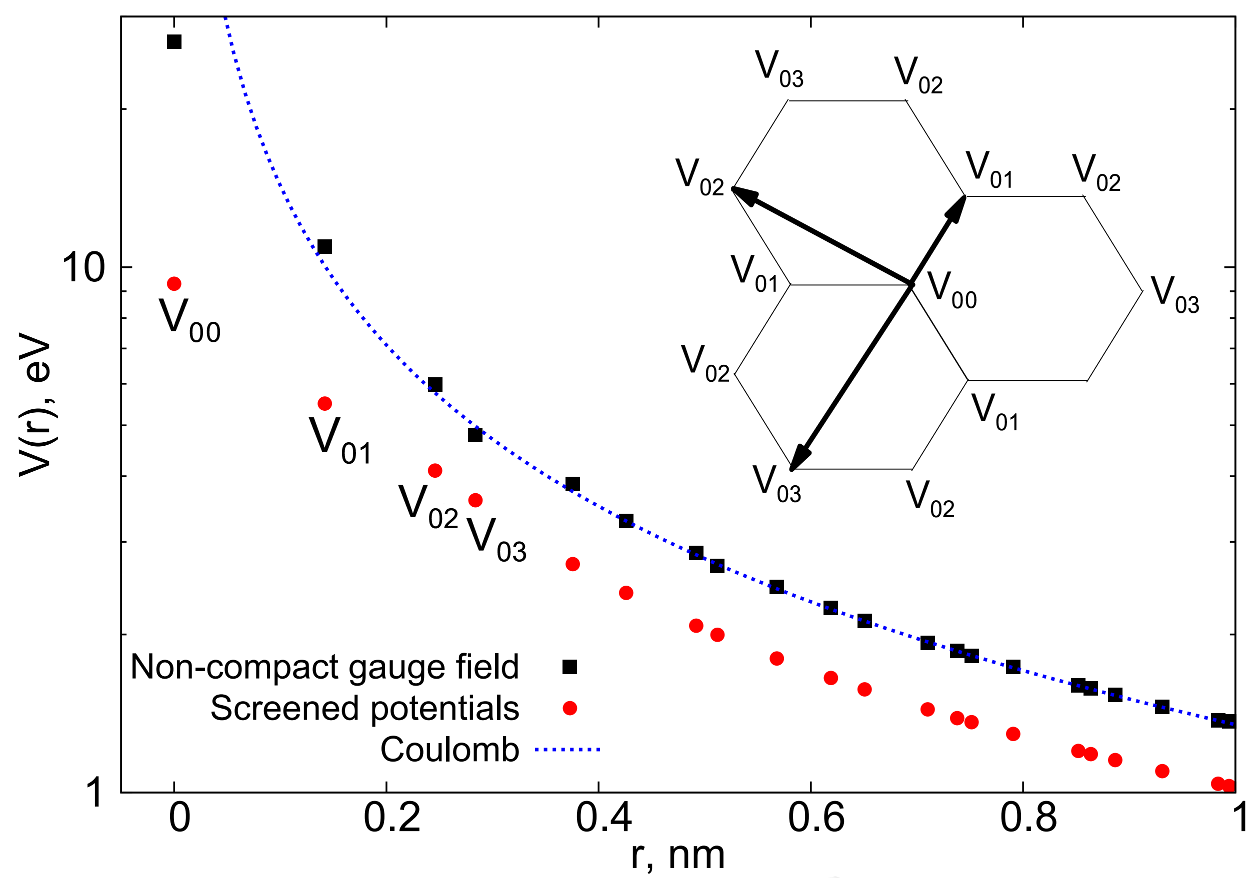
$$H_1 = \sum_{\vec{X},\vec{Y},\sigma,\sigma'} n_\sigma(\vec{X}) \left[\frac{U}{2}\delta_{\vec{X},\vec{Y}} + \frac{e^2(1-\delta_{\vec{X},\vec{Y}})}{4\pi|\vec{X}-\vec{Y}|} \right] n_{\sigma'}(\vec{Y})$$

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

- ***ab initio*** parameters:

		graphene		graphite	
		bare	cRPA	bare	cRPA
U	(eV)	17.0	9.3	17.5, 17.7	8.0, 8.1
V_1	(eV)	8.5	5.5	8.6	3.9
V_2	(eV)	5.4	4.1	5.4, 5.4	2.4, 2.4
V_3	(eV)	4.7	3.6	4.7	1.9

Wehling et al. (2011)



Ulybyshev et al. (2013)

- other *ab initio* methods: QC-PPP, Thomas-Fermi

Honeycomb fermions & **many-body interactions**

- **Hamiltonian:** *tight-binding part* + *interaction part* $H = H_0 + H_1$

- **What to expect from many-body interaction effects?**

  - Dirac materials qualitatively different from normal metals:

    - lack of electric screening

    - renormalisation of Fermi velocity

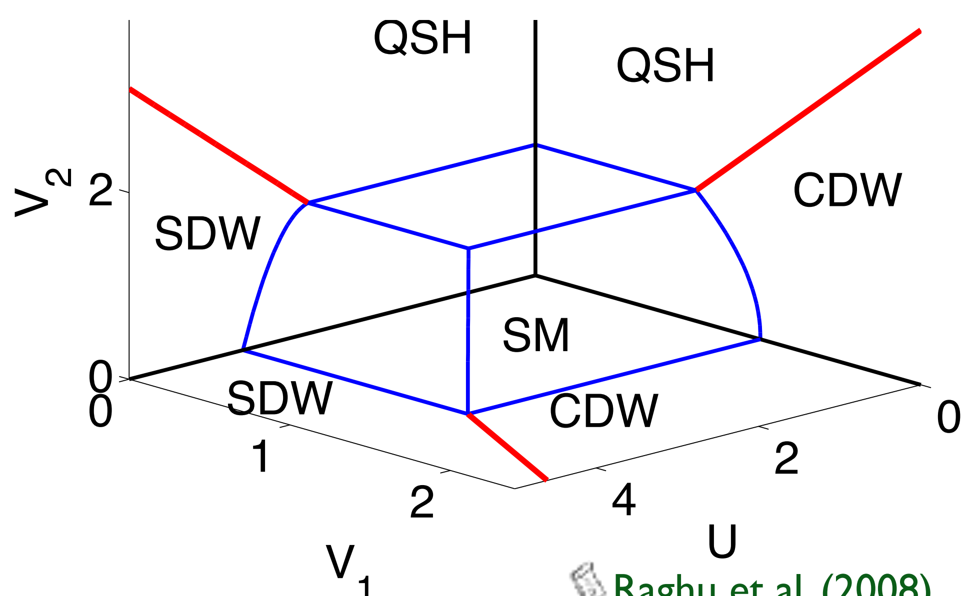
  - **dynamical generation of mass gaps?**

    - triggered by strong short-ranged i.a. components

    - Dirac fermions have vanishing DOS at Fermi level

    - critical interaction strength for transition

mean-field phase diagram:



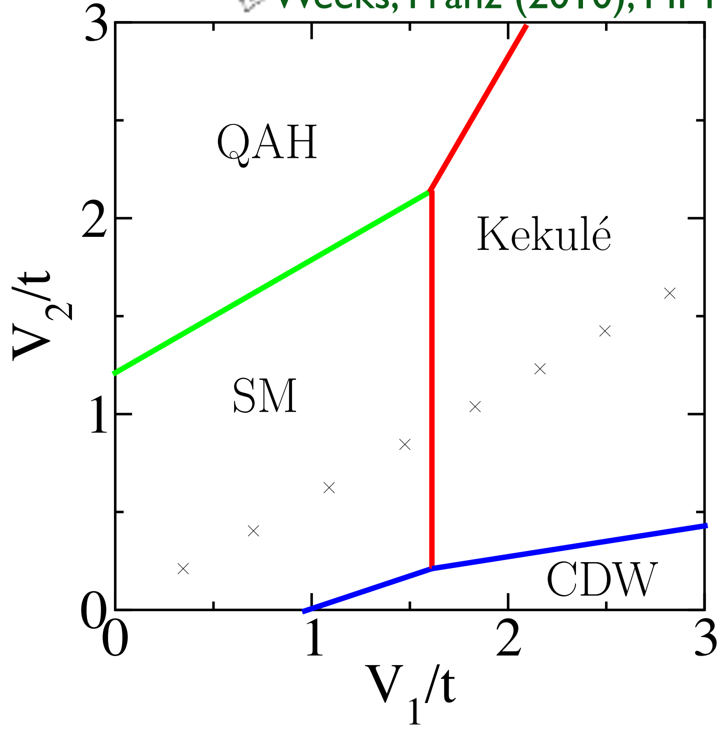
Raghu et al. (2008)

  - **Experimental studies:** graphene is in SM phase!

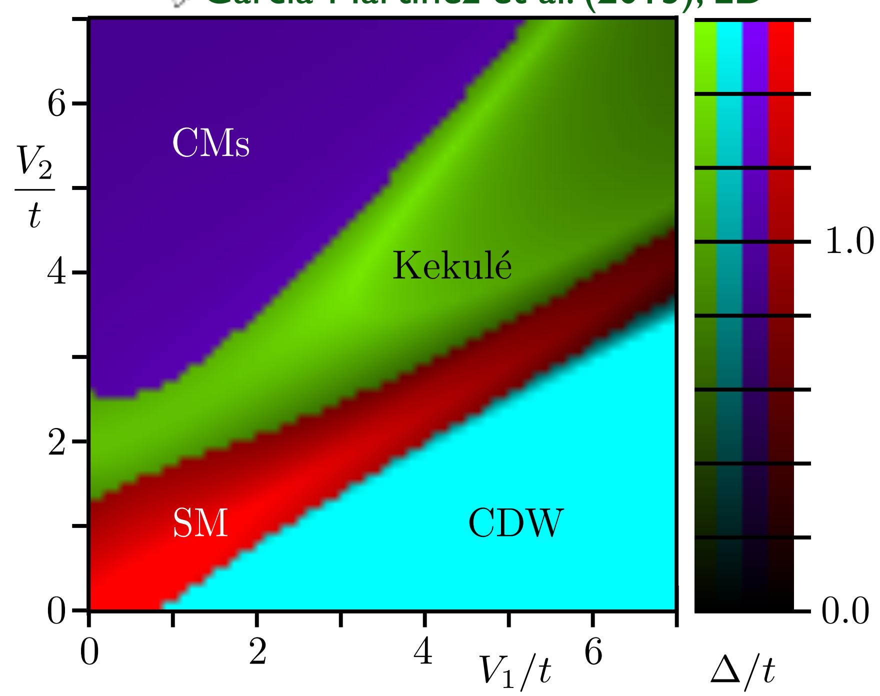
Refined phase diagrams - **spinless** fermions on the honeycomb

- **short-ranged** interaction components **V_1, V_2**

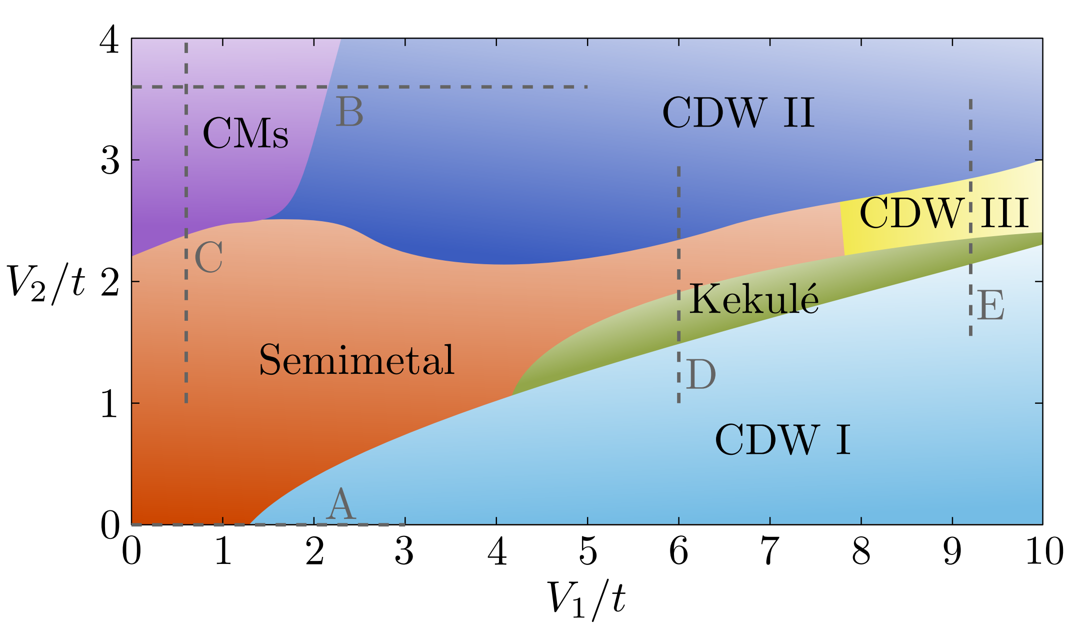
Weeks, Franz (2010), MFT



Garcia-Martinez et al. (2013), ED



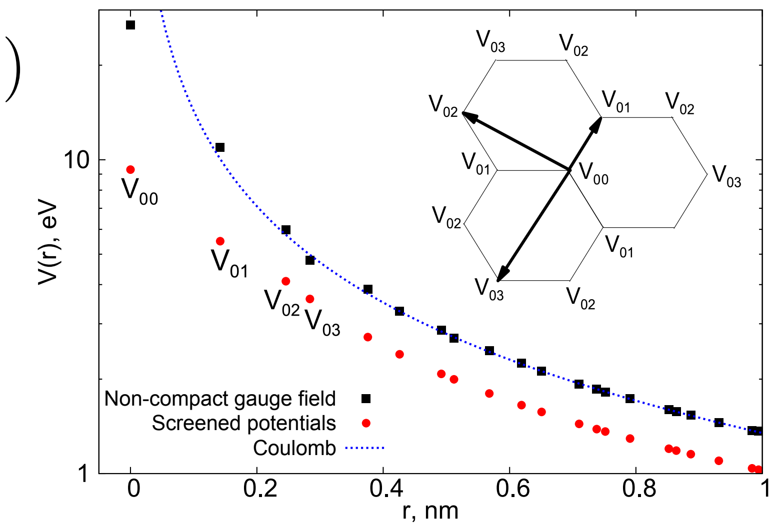
Motruk et al. (2015), DMRG



- many more suggestions…
- competition of many phases!
- various **ordering transitions**

Long-range tail

- **use cRPA values & long-range extrapolation** $\sim 1/(\epsilon_\sigma\, r)$



  - for fast enough decay of long-range tail: $\epsilon_\sigma \approx 1.41$
    - ➡ study **AFM ground state** with QMC methods
    - ➡ compatible with semimetallic ground state

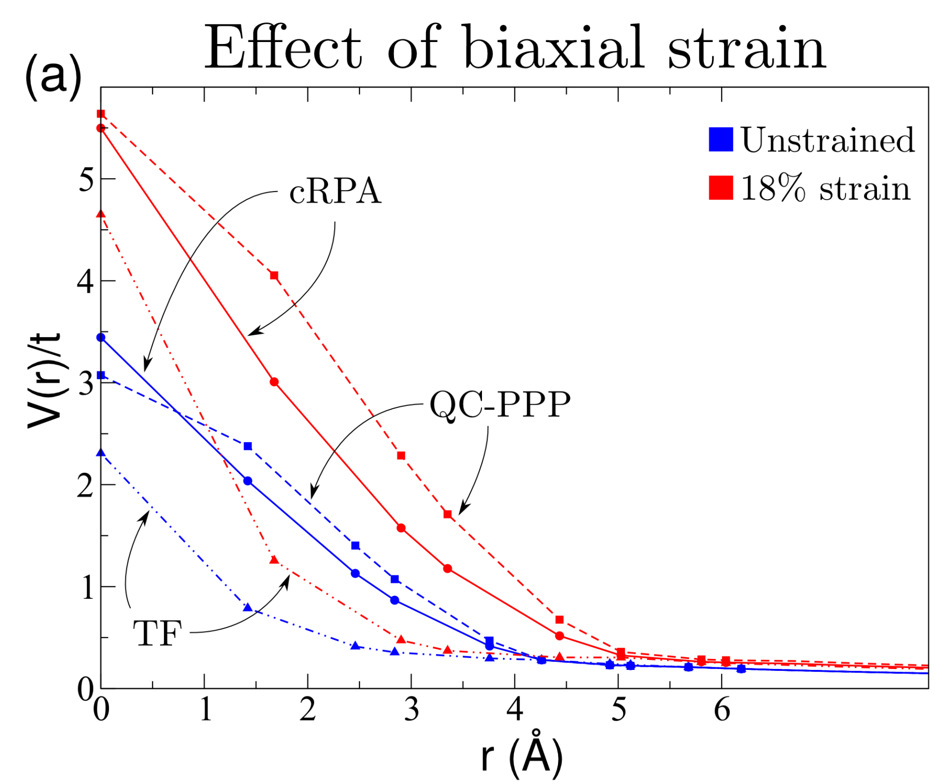
Ulybyshev et al. (2013)
Smith & von Smekal (2014)

  - hybrid-MC: hints for CDW transition in U-V plane

Buividovich, Smekal, Smith, Ulybyshev (2016)

- **interaction-driven metal-insulator transition in strained graphene** Tang et al. (2015)

  - AFM transition for TF parameters at 18% strain
  - data of cRPA parameters not conclusive
  - sign problem for |t'| > 0
  - sign problem for QC-PPP data



Interim summary

- electrons in neutral suspended unstrained graphene: **semimetallic** state
- *ab initio* parameters & models: **vicinity to interaction-induced** phase transition
- **different ordering transitions** may be induced by interaction parameters
    - AFM, CDW, CM, Kekulé,…

✦ **Theoretical methods:**

- *MFT: not exact, no correlations between different channels, no accurate critical exponents*
- *QMC: exact but sign problem if long-range tail falls off too slowly - bias towards AFM state*
- *ED: exact but too expensive for spin-1/2*
- ***(F)RG:** all correlation channels, numerically feasible, no sign problem, critical exponents*
    - **fermion FRG**: unbiased determination of many-body instabilities

      with Sánchez de la Peña, Lichtenstein, Honerkamp
    - **fermion-boson FRG**: critical exponents, calculation in SSB phase

      with Torres, Classen, Herbut

(I) Many-body **instabilities** of graphene's Dirac electrons

from the functional Renormalization group

with D. Sánchez de la Peña, J. Lichtenstein, and C. Honerkamp

Effective action

- system of interacting fermions: $\mathcal{S}[\psi,\bar\psi] = -(\bar\psi, G_0^{-1}\psi) + V[\psi,\bar\psi]$

general two-particle i.a.

- bare propagator (translation and spin rotation invariance):

single-particle energy

$$G_0(k_0,\mathbf{k}) = \frac{1}{ik_0 - \xi_\mathbf{k}}, \quad \xi_\mathbf{k} = \epsilon_\mathbf{k} - \mu$$

- generating functional (for connected Green functions):

$$\mathcal{G}[\eta,\bar\eta] = -\ln \int \mathcal{D}\psi\mathcal{D}\bar\psi\, e^{\mathcal{S}[\psi,\bar\psi]} e^{(\bar\eta,\psi)+(\bar\psi,\eta)}$$

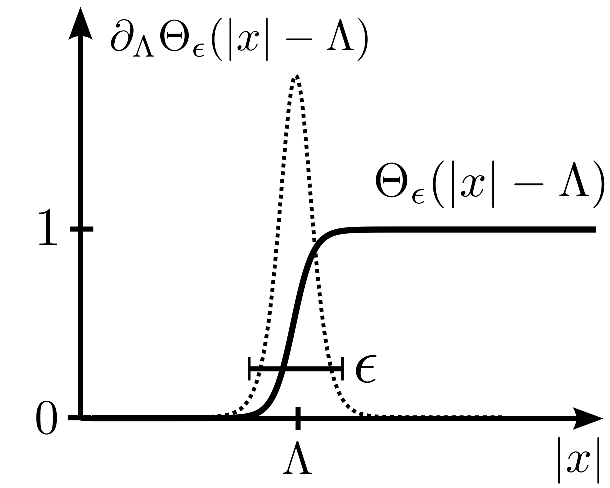
- effective action: $\Gamma[\phi,\bar\phi] = (\bar\eta,\phi) + (\bar\phi,\eta) + \mathcal{G}[\eta,\bar\eta], \quad \phi = -\dfrac{\partial\mathcal{G}}{\partial\bar\eta}, \quad \bar\phi = \dfrac{\partial\mathcal{G}}{\partial\eta}$

(generates one-particle irreducible vertex functions)

Functional **flow equations**

- modify bare propagator by introduction of flow parameter

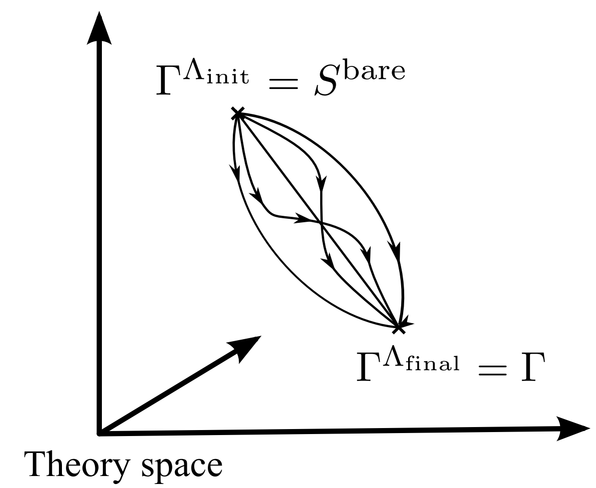
  (IR cutoff, cuts out soft modes $<\Lambda$): $G_0^\Lambda(k_0,\mathbf{k}) = \frac{\Theta_\epsilon(|\xi_\mathbf{k}|-\Lambda)}{ik_0-\xi_\mathbf{k}}$



- define all the above quantities with modified bare propagator

  → variation w.r.t to scale provides **exact RG equation**:

$$\frac{\partial}{\partial\Lambda}\Gamma^\Lambda[\phi,\bar\phi] = \mathrm{Tr}\left[G_0^\Lambda\frac{\partial(G_0^\Lambda)^{-1}}{\partial\Lambda}\right] - \mathrm{Tr}\left[\left(\frac{\delta^2\Gamma^\Lambda[\phi,\bar\phi]}{\delta\phi\delta\bar\phi}+(G_0^\Lambda)^{-1}\right)^{-1}\frac{\partial(G_0^\Lambda)^{-1}}{\partial\Lambda}\right]$$



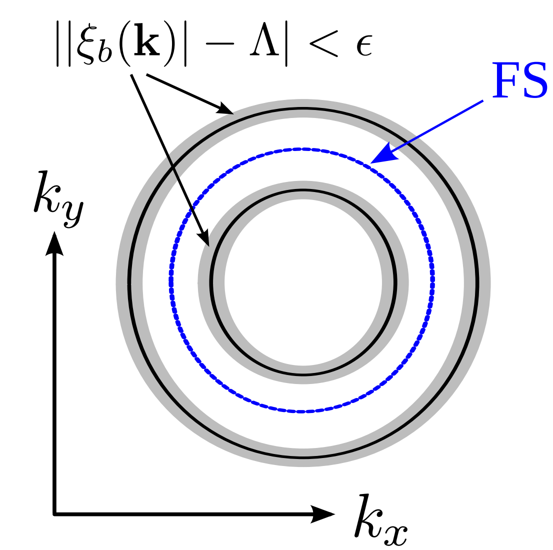
Wetterich (1993)

Salmhofer & Honerkamp (2001)

- exact RG equation has one-loop structure

- removing cutoff ($\Lambda\to 0$) yields the full effective action

- lowering cutoff corresponds to momentum-shell integration



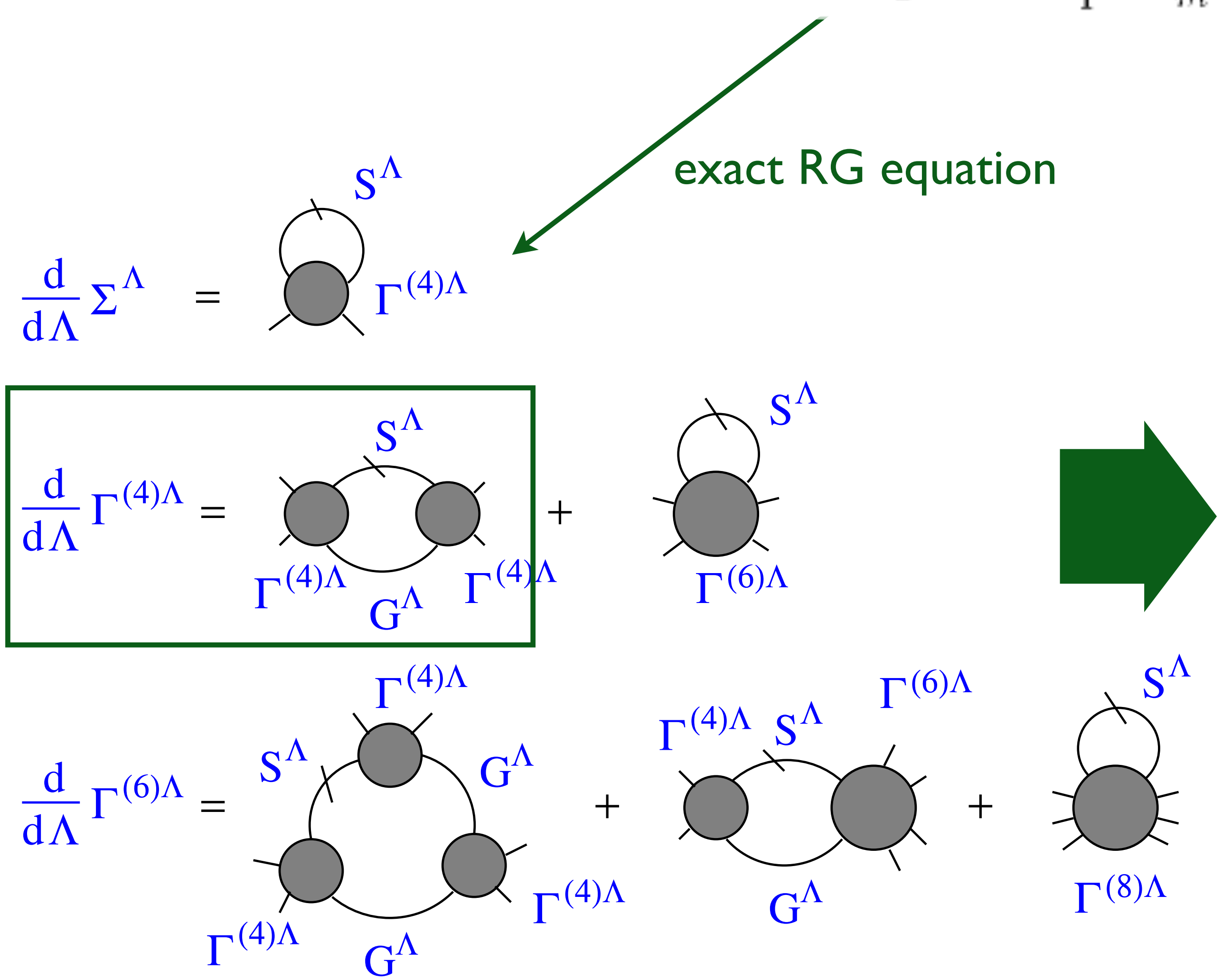
from Platt, Hanke, Thomale (2013)

Truncation & Approximations

- exact RG equation cannot be solved exactly!

- starting point for systematic approximations (vertex expansion)

$$\Gamma^{\Lambda}[\phi,\bar{\phi}] = \sum_{m=0}^{\infty} \frac{1}{(m!)^2} \sum_{K_1 \dots K_m} \sum_{K'_1 \dots K'_m} \gamma_m^{\Lambda}(K'_1,\dots,K'_m;K_1,\dots,K_m) \prod_{j=1}^{m} \bar{\phi}_{K'_j}\phi_{K_j}$$



- neglect 6-point and higher vertices
- neglect self-energy feedback

Salmhofer & Honerkamp (2001)

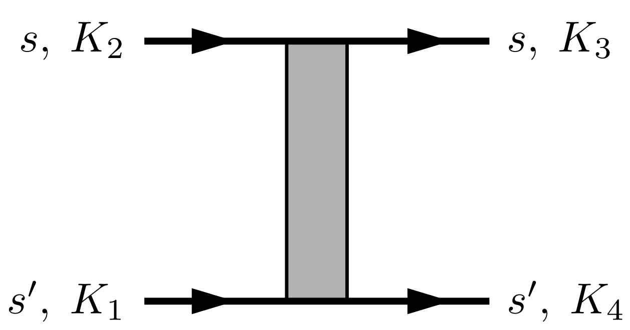
… infinite hierarchy of flow equations!

Symmetries & Approximations

- system with **spin-rotational invariance**:

  - RG flow of general 4-point function $\Gamma^{(4)\Lambda}$: $\Gamma^{(4)\Lambda}_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} = V^{\Lambda}\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4} - V^{\Lambda}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}$

    ➡ **interaction vertex *V*^Λ**:



$$V_{\Lambda}(k_1, k_2, k_3, k_4)$$

- momentum arguments include *frequency*, *wavevector* and *orbital* indices

- ground-state properties: neglect frequency dependence, set external frequencies to zero

Symmetries & Approximations

- system with **spin-rotational invariance**:

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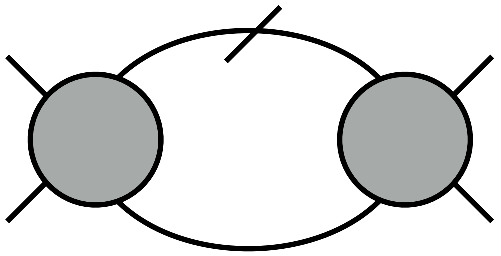
    ➡ flow of **spin-independent interaction vertex *V*^Λ**:

$$\begin{aligned}\frac{d}{d\Lambda}V^\Lambda(K_1,K_2;K_3,K_4) = &\int dK\, V^\Lambda(K_1,K_2,K)\, L^\Lambda(K,-K+K_1+K_2)\, V^\Lambda(K,-K+K_1+K_2,K_3)\,,\\ &+\int dK \Big[-2V^\Lambda(K_1,K,K_3)\, L^\Lambda(K,K+K_1-K_3)\, V^\Lambda(K+K_1-K_3,K_2,K)\\ &\quad +V^\Lambda(K_1,K,K+K_1-K_3)\, L^\Lambda(K,K+K_1-K_3)\, V^\Lambda(K+K_1-K_3,K_2,K)\\ &\quad +V^\Lambda(K_1,K,K_3)\, L^\Lambda(K,K+K_1-K_3)\, V^\Lambda(K_2,K+K_1-K_3,K)\Big]\,,\\ &+\int dK\, V^\Lambda(K_1,K+K_2-K_3,K)\, L^\Lambda(K,K+K_2-K_3)\, V^\Lambda(K,K_2,K_3)\,.\end{aligned}$$

  - where $L^\Lambda(K,K') = \dfrac{d}{d\Lambda}[G_0^\Lambda(K)G_0^\Lambda(K')]$



Symmetries & Approximations

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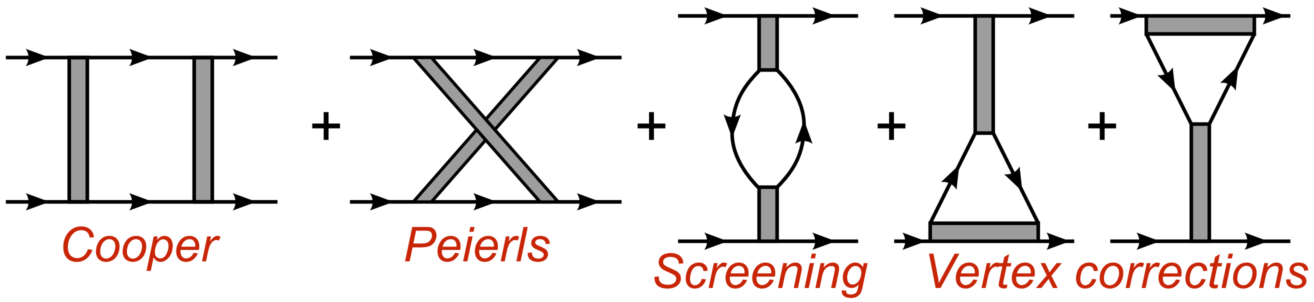
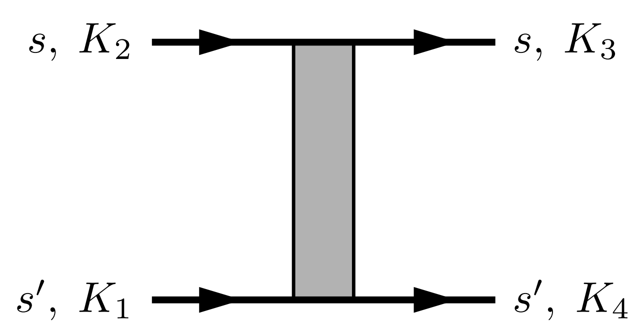
    ➡ flow of **spin-independent interaction vertex *V*^Λ**:

$$\frac{d}{d\Lambda} V^\Lambda(K_1, K_2; K_3, K_4) =$$



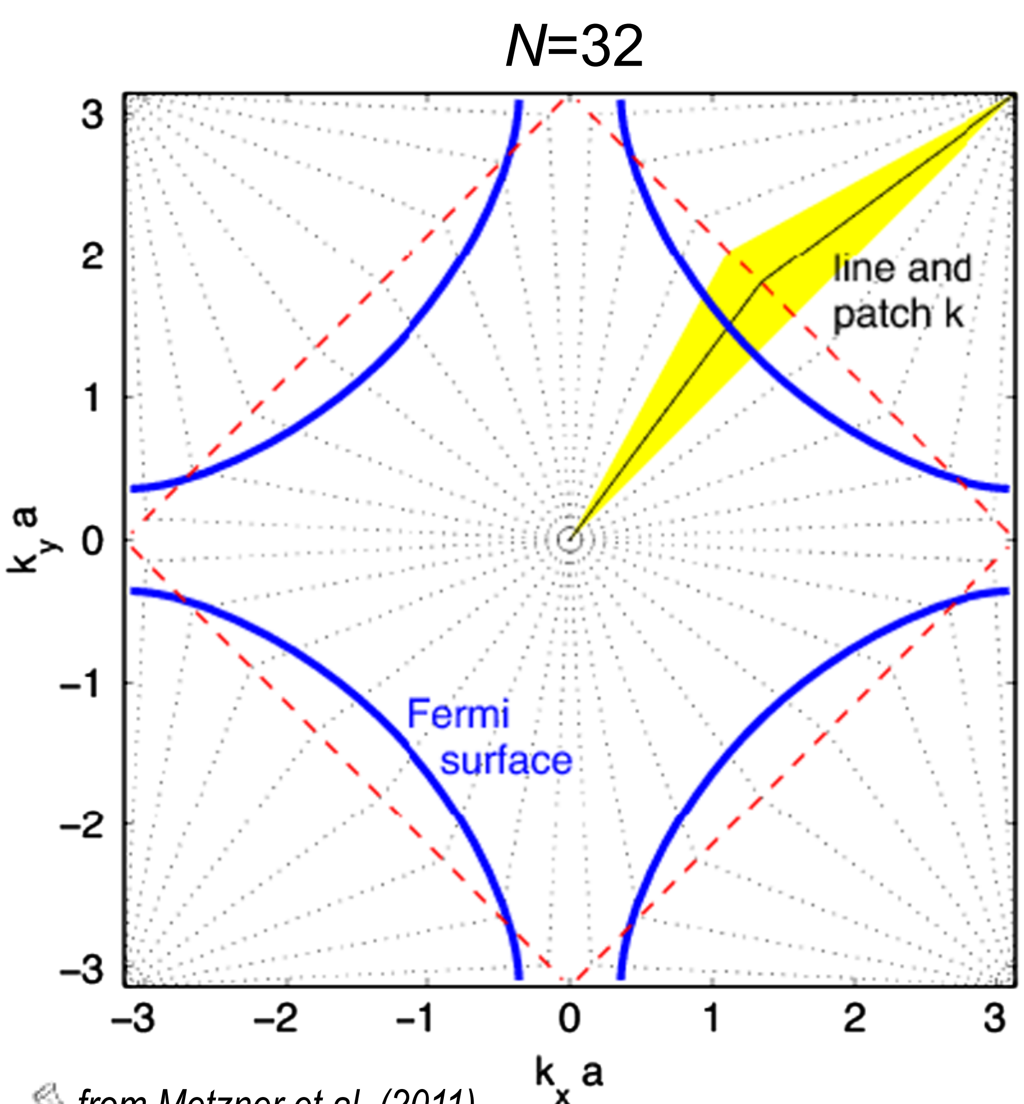
- corresponds to *infinite order summation* of one-loop *pp* and *ph* terms
- unbiased investigation of competition between various correlations
- **flow to strong coupling** indicates **ordering transition**: analyze components of V^Λ

Fermi-surface patching scheme



$$V_\Lambda(k_1, k_2, k_3, k_4)$$

- wavevector dependence of **Fermi surface** from discretization in ***N* patches:**

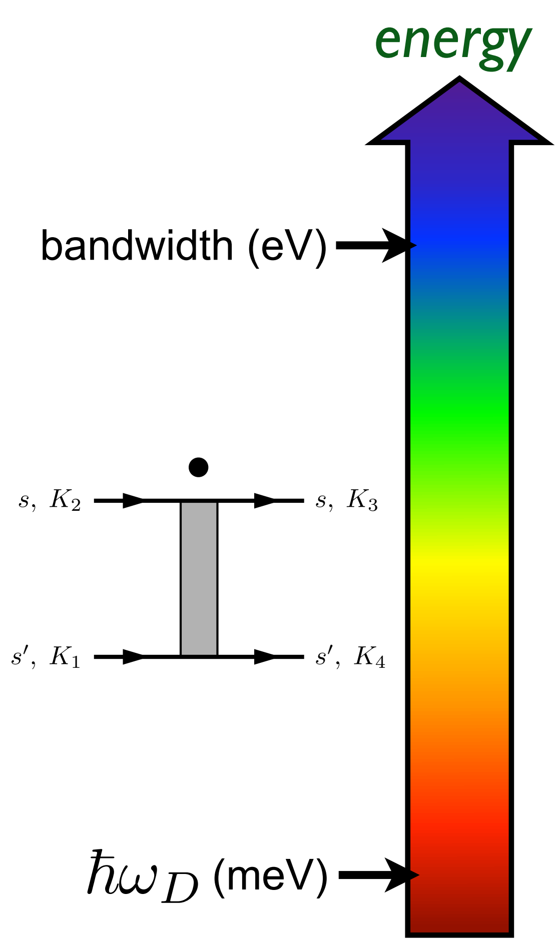


from Metzner et al. (2011)

- **interaction constant within one patch**
- representative momenta lie at Fermi level
- **finite set of coupled flow equations** for components of *V*^
- facilitates numerical implementation
- **example:**
  - *t*-*t'*-*μ*-Hubbard model on the square lattice: vertex has N^3 components
  - generally: ***V*^ has $N_b^4 N^3$ components**

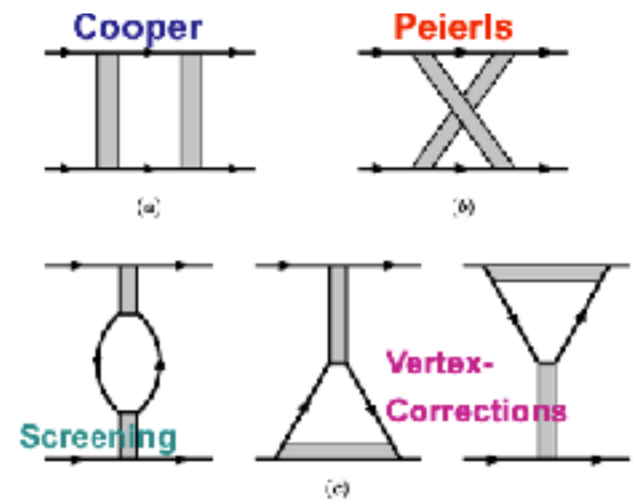
fRG: from **bare** to **effective interaction**

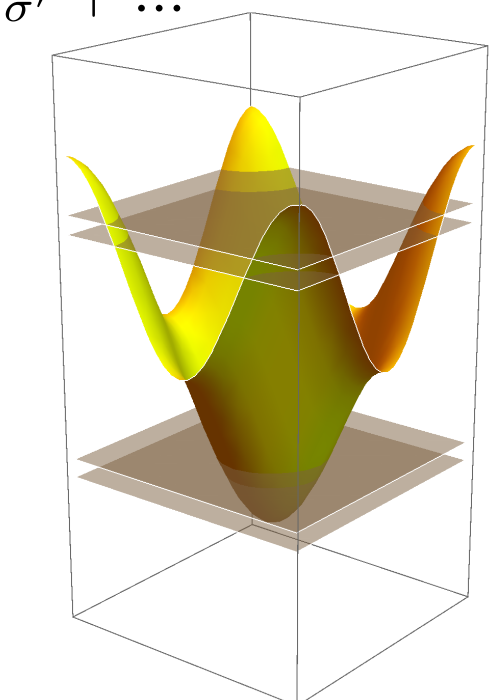
- excitations at intermediate scales generate momentum structure in low-energy interaction



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

fRG:

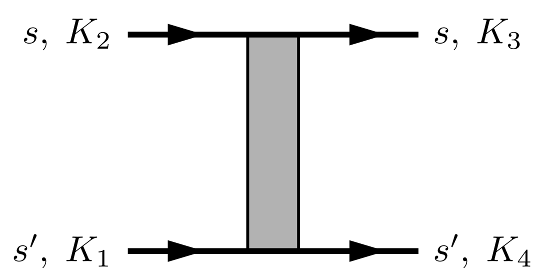




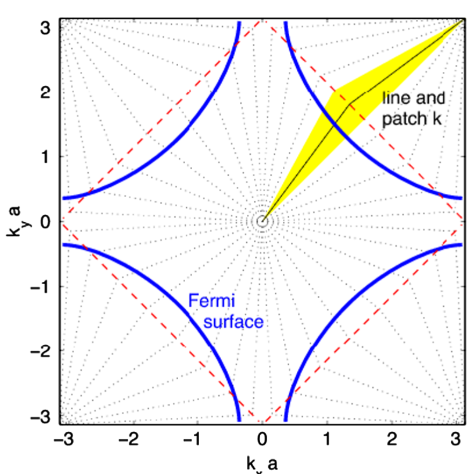
$$H_{\text{eff}} = \frac{1}{2} \sum_{\vec{p},\vec{p}',\vec{q},s,s'} V(\vec{p},\vec{p}',\vec{p}+\vec{q})\, c^\dagger_{\vec{p}+\vec{q},s} c^\dagger_{\vec{p}'-\vec{q},s'} c_{\vec{p}',s'} c_{\vec{p},s}$$

- low-energy effective action & momentum structure
  - ➡ two-particle interaction vertex $V(\vec{p},\vec{p}',\vec{p}+\vec{q})$
  - ➡ flow to strong coupling: singularity for $\Lambda \to \Lambda^*$
  - ➡ read off dominant interactions and e.g. extract form factors of order parameters

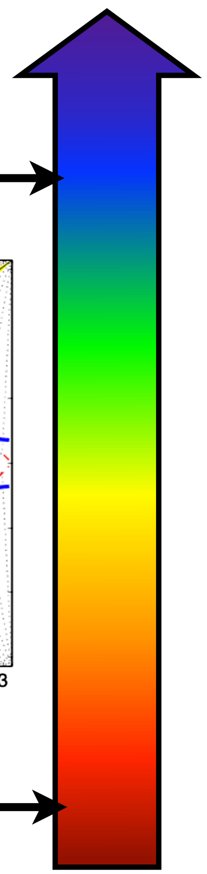
fRG: from **bare** to **effective interaction**



- sharp momentum structures in the interaction vertex emerge
- e.g., onsite interaction (U=3.0t), typical pattern (k_3 fixed at point 1):



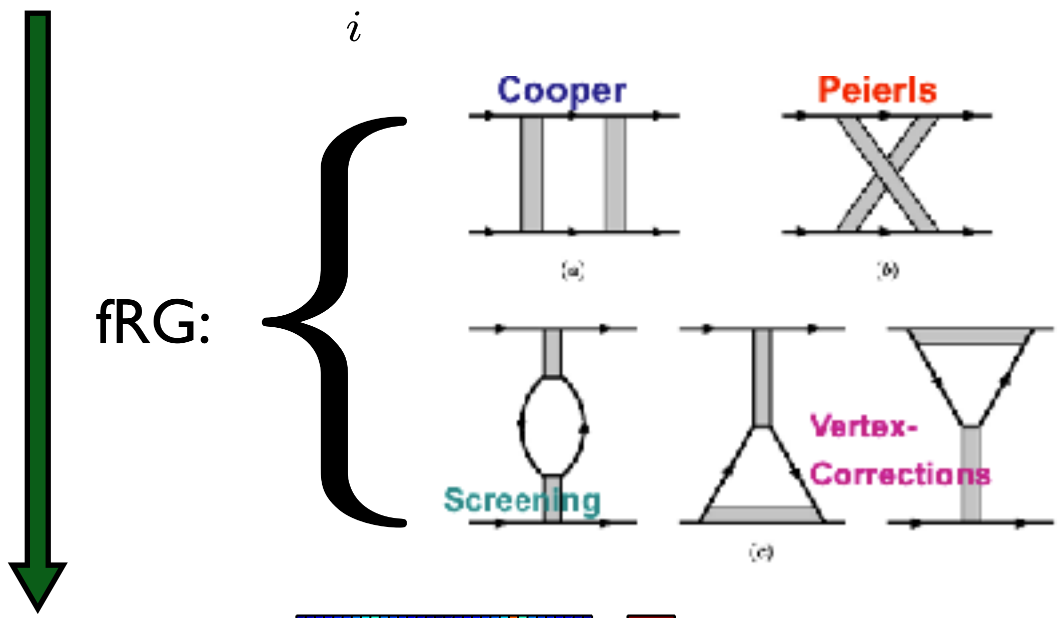
bandwidth (eV)



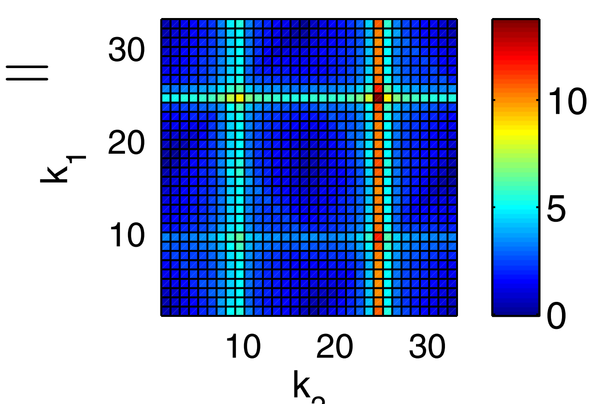
$\hbar\omega_D$ (meV)

$$H_{\text{bare}} = U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

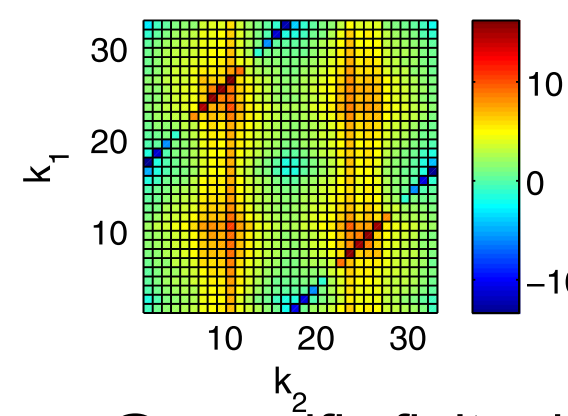
fRG:



$H_{\text{eff}} =$



or H_{eff} =



@ zero doping

@ specific finite doping

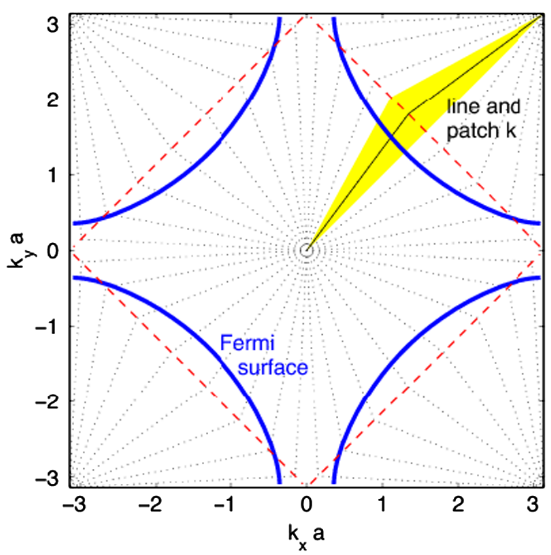
$$J\sum_{\langle i,j\rangle} e^{i\mathbf{Q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\mathbf{S}_i\cdot\mathbf{S}_j$$

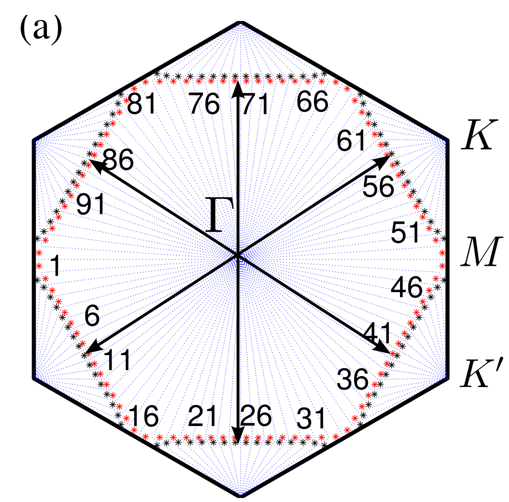
$$H^{\Lambda}_{dSC} = V_{dSC}\sum_{\mathbf{k},\mathbf{k}'} d(\mathbf{k})d(\mathbf{k}')c^{\dagger}_{\mathbf{k}',\uparrow}c^{\dagger}_{-\mathbf{k}',\downarrow}c_{-\mathbf{k},\downarrow}c_{\mathbf{k},\uparrow}$$

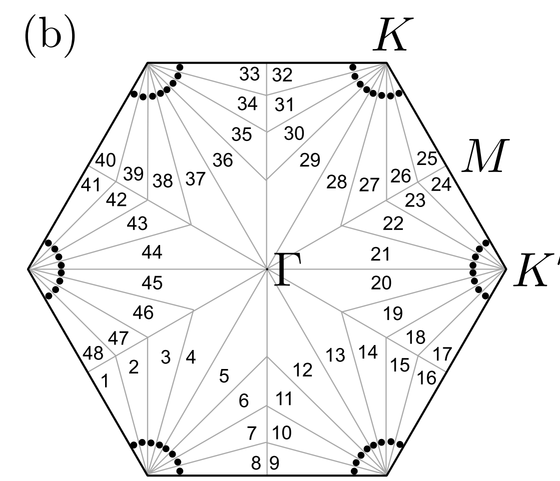
- mean-field decoupling → antiferromagnetic SDW (**AF-SDW**) or ***d*-wave SC**

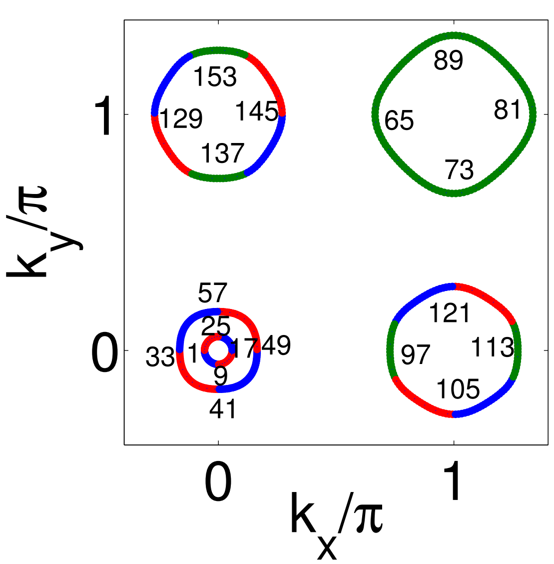
Application to various systems

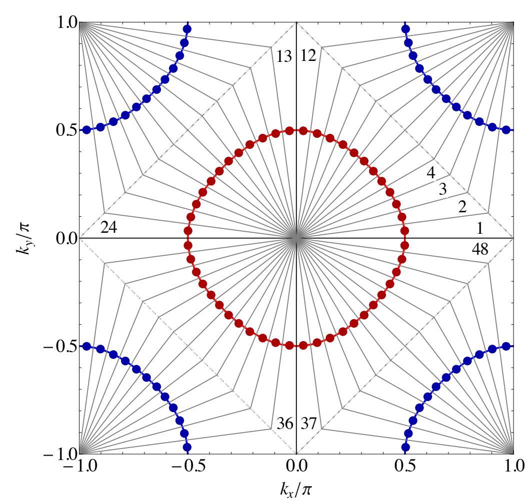
- **Fermi-surface patching scheme:**
  - provides effective interaction without a priori assumption on SB pattern
  - includes interplay of scale- & momentum-dependent scattering processes
  - versatile tool for elaborate microscopic structures and multiple bands (DFT)









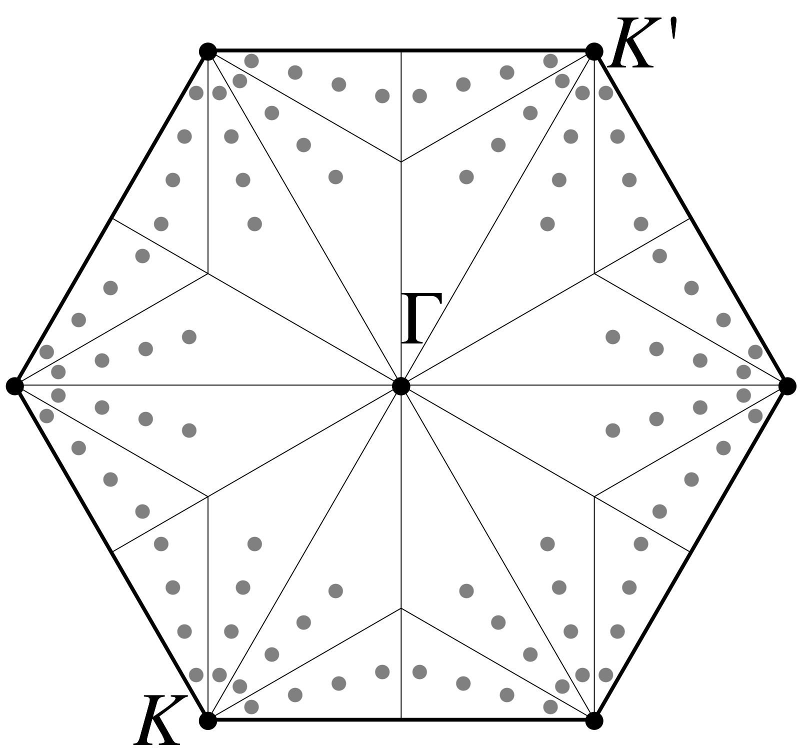


- *Honerkamp & Salmhofer (2001,2003)*
- *Kuroki et al. (2008)*
- *Wang et al. (2009,2010)*
- *Thomale et al. (2011,2013)*
- *Raghu et al. (2008)*
- *Scherer et al. (2011,2012)*
- *Lichtenstein et al. (2014)*
- *...*

  - exhibits AF, F, CDW, CDW_3, *d*SC, *s*SC, *f*SC, QSH, cBO, sBO…

fermion FRG: **key features**

- **Disovery tool** for many-body instabilities in correlated many-fermion systems
  - treats all fermionic fluctuation channels on **equal footing**
  - **infinite-order resummation** of all fermionic 1-loop diagrams
  - unbiased identification of leading instability in presence of **competing correlations**
  - due to truncations/approximations: **qualitative** (not quantitative) tool



- **Challenge:** discretization of $V(\vec{p}, \vec{p}', \vec{p}+\vec{q})$
  - **long-range Coulomb tail**: sufficient resolution of wave-vector dependence required!
  - **FS patching**: vertex function depends on three wave-vector variables - expensive!
    - cubic scaling with patch points ~ N^3

Channel **decomposition**

- Singular contributions produced for specific **transfer momenta**
  - parametrize coupling function by decomposition into single channel coupling functions

initial bare i.a.

$$V^{\{b_i\}}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3) = V^{(0),\{b_i\}}_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} - \Phi^{\mathrm{SC},\{b_i\}}_{\mathbf{k}_1+\mathbf{k}_2,\frac{\mathbf{k}_1-\mathbf{k}_2}{2},\frac{\mathbf{k}_4-\mathbf{k}_3}{2}} + \Phi^{\mathrm{C},\{b_i\}}_{\mathbf{k}_1-\mathbf{k}_3,\frac{\mathbf{k}_1+\mathbf{k}_3}{2},\frac{\mathbf{k}_2+\mathbf{k}_4}{2}} + \Phi^{\mathrm{D},\{b_i\}}_{\mathbf{k}_3-\mathbf{k}_2,\frac{\mathbf{k}_1+\mathbf{k}_4}{2},\frac{\mathbf{k}_2+\mathbf{k}_3}{2}},$$

transfer momenta

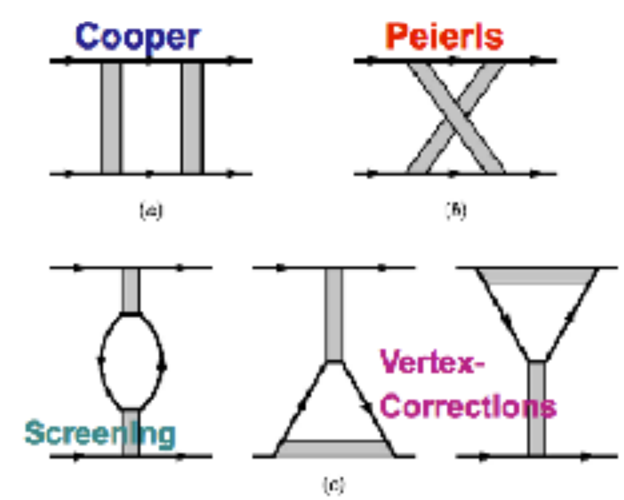
  - Φ generated during flow:

$$\dot\Phi^{\mathrm{SC},\{b_i\}}_{\mathbf{k}_1+\mathbf{k}_2,\frac{\mathbf{k}_1-\mathbf{k}_2}{2},\frac{\mathbf{k}_4-\mathbf{k}_3}{2}} = -\mathcal{T}^{\{b_i\}}_{\mathrm{pp}}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)\,,$$

$$\dot\Phi^{\mathrm{C},\{b_i\}}_{\mathbf{k}_1-\mathbf{k}_3,\frac{\mathbf{k}_1+\mathbf{k}_3}{2},\frac{\mathbf{k}_2+\mathbf{k}_4}{2}} = \mathcal{T}^{\mathrm{cr},\{b_i\}}_{\mathrm{ph}}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)\,,$$

$$\dot\Phi^{\mathrm{D},\{b_i\}}_{\mathbf{k}_3-\mathbf{k}_2,\frac{\mathbf{k}_1+\mathbf{k}_4}{2},\frac{\mathbf{k}_2+\mathbf{k}_3}{2}} = \mathcal{T}^{\mathrm{d},\{b_i\}}_{\mathrm{ph}}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)\,.$$

Husemann & Salmhofer (2008)



  - strong dependence on transfer momentum is kept as if carried by exchange boson
  - weak dependences captured by expansion in form factors:

strong variable *weak variable*

$$\Phi^{\mathrm{SC}}_{\mathbf{l},\mathbf{k},\mathbf{k}'} \approx \sum_{m,n} f_m(\mathbf{k}) f_n(\mathbf{k}') P_{m,n}(\mathbf{l})$$

bosonic propagator

$$P_{m,n}(l) = \hat P\left[\Phi^{\mathrm{SC}}\right]_{m,n}(l) = \int d\mathbf{k}\,d\mathbf{k}'\,f_m(\mathbf{k})\,f_n(\mathbf{k}')\,\Phi^{\mathrm{SC}}_{l,k,k'}$$

  - rewrite flow in term of three bosonic propagators $P(l)$, $C(l)$, $D(l)$

functional RG: **interaction vertex**

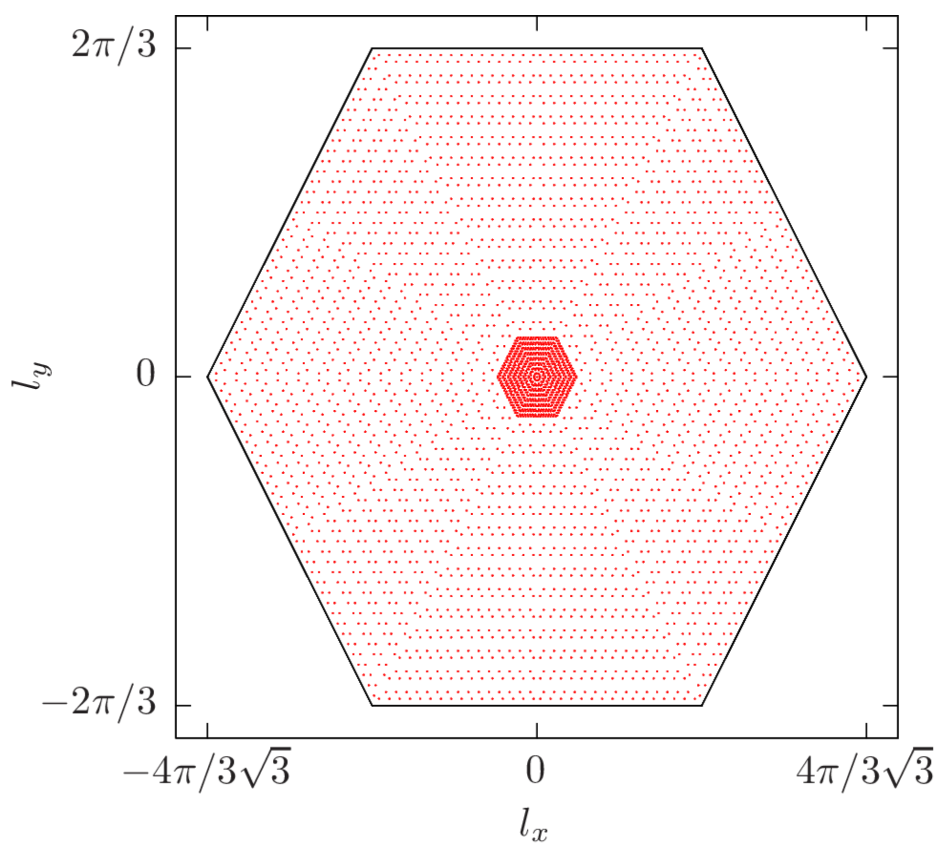
- employ full-HD wavevector resolution of interaction vertex

$$V(\vec{k}_1,\vec{k}_2,\vec{k}_3) = V^{(0)}_{\vec{k}_1,\vec{k}_2,\vec{k}_3} - \Phi^{\mathrm{SC}}_{\vec{k}_1+\vec{k}_2,\frac{\vec{k}_1-\vec{k}_2}{2},\frac{\vec{k}_4-\vec{k}_3}{2}} - \Phi^{\mathrm{C}}_{\vec{k}_1-\vec{k}_3,\frac{\vec{k}_1+\vec{k}_3}{2},\frac{\vec{k}_2+\vec{k}_4}{2}} + \Phi^{\mathrm{D}}_{\vec{k}_3-\vec{k}_2,\frac{\vec{k}_1+\vec{k}_4}{2},\frac{\vec{k}_2+\vec{k}_3}{2}}$$

transfer momenta

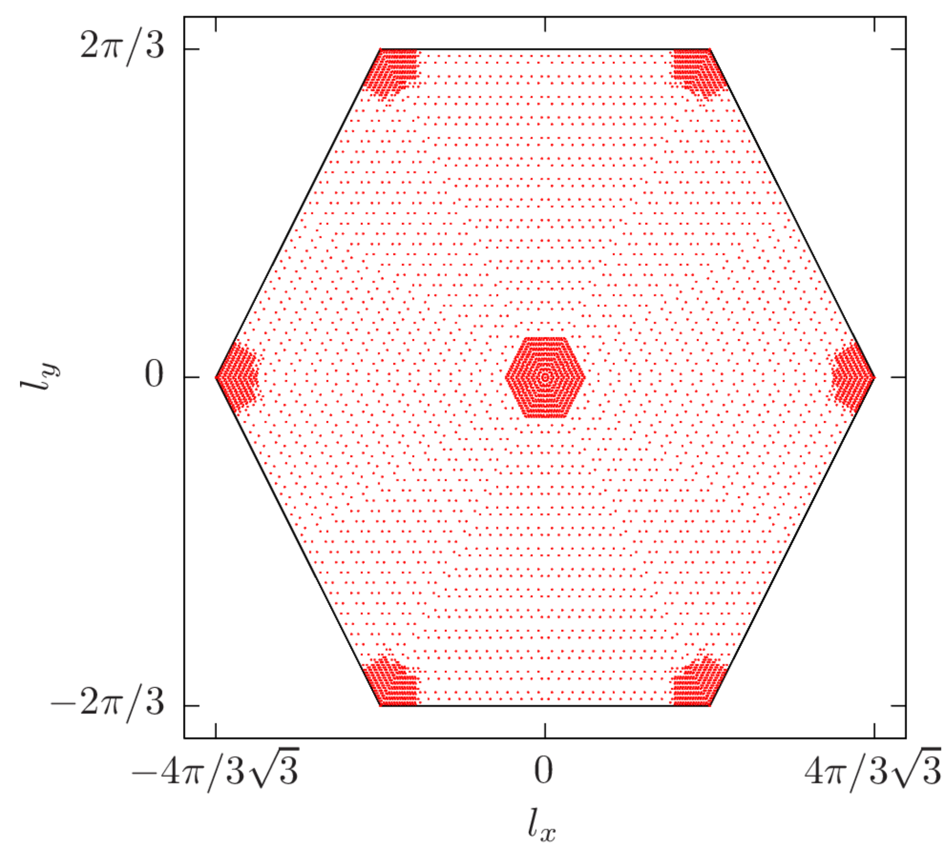
- *Brillouin zone mesh for transfer momenta:*

PP channel



$P^{b_{1\ldots4}}_{m,n}(\vec{l})$: 3217 transfer momenta

PH channel

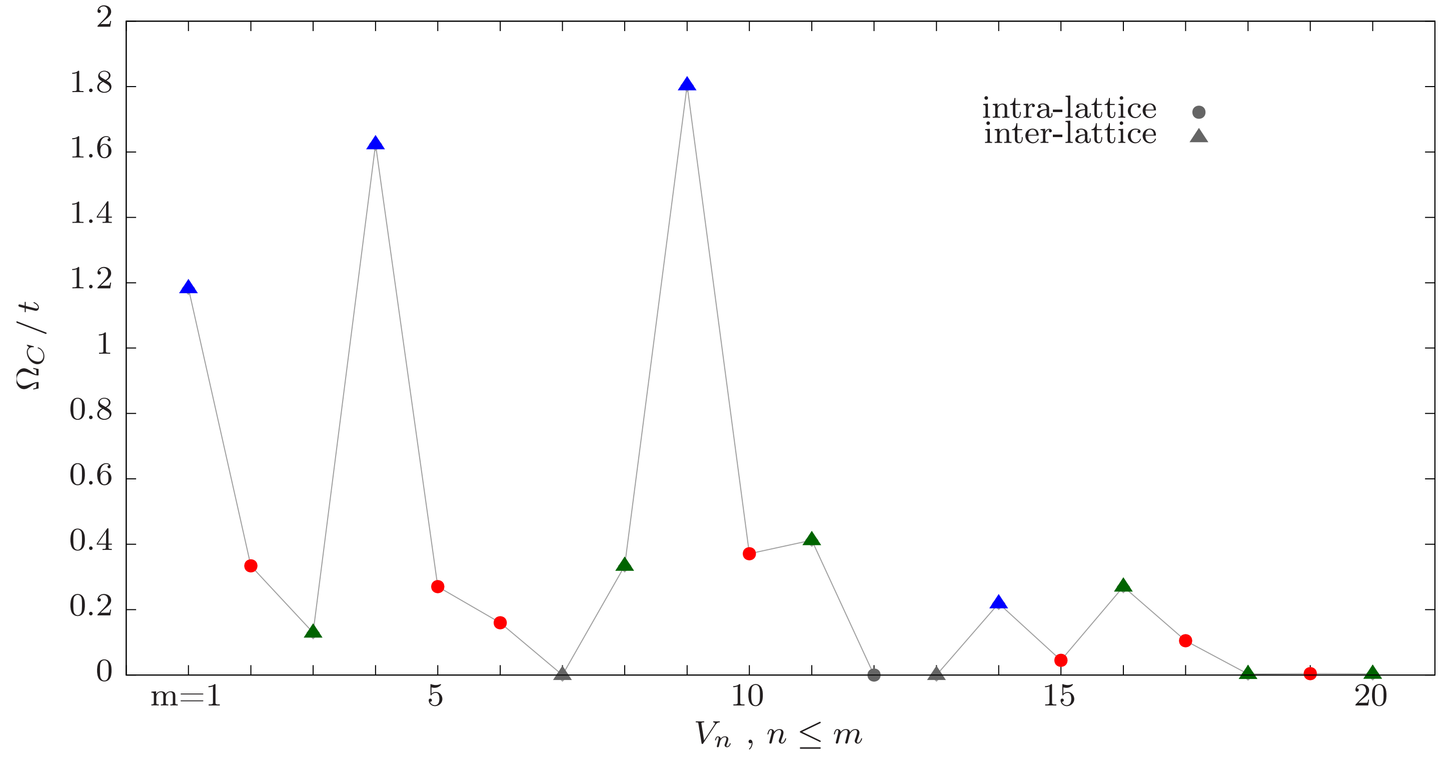


$D^{b_{1\ldots4}}_{m,n}(\vec{l}),\ C^{b_{1\ldots4}}_{m,n}(\vec{l})$: 3661 transfer momenta

- *expand weak momentum dependencies in basis of lattice harmonics*
- *efficient calculations on a large number of **multi-core CPUs***

HD-fRG calculations - **results**

- **competing interactions:**
  - successively include more i.a. terms
  - choose values according to cRPA
  - different types of charge order

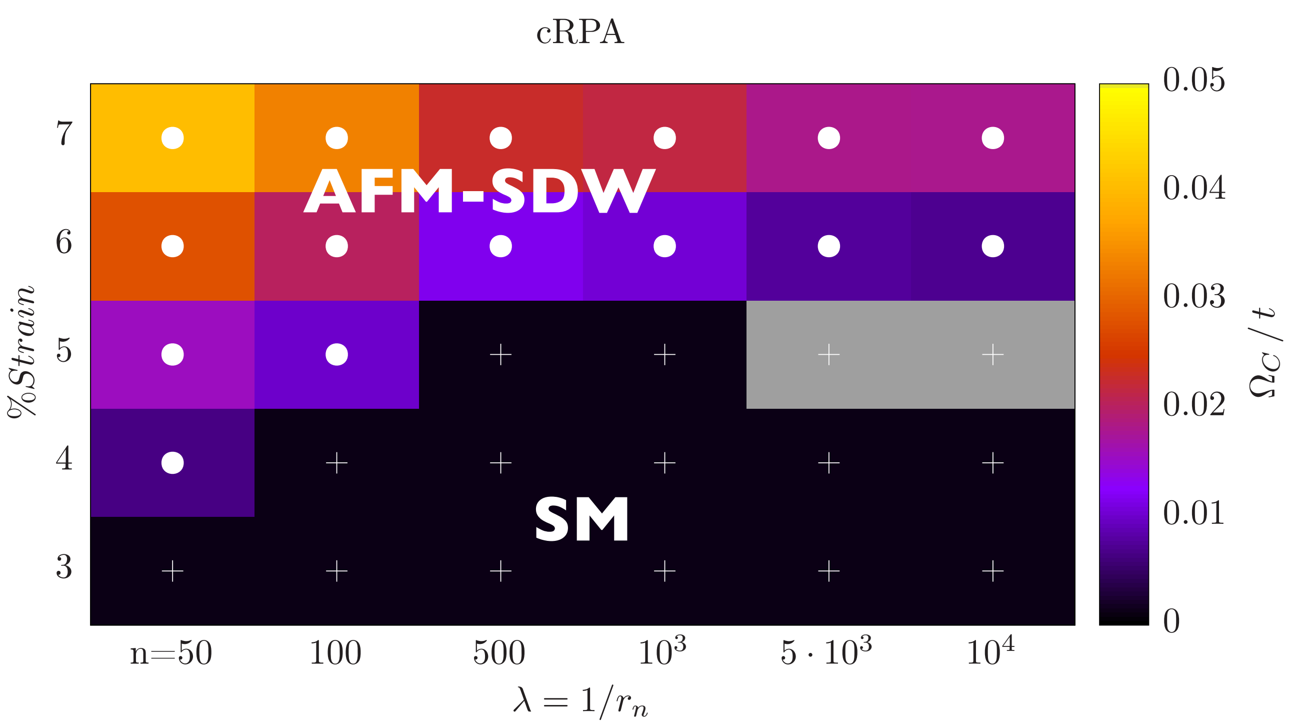


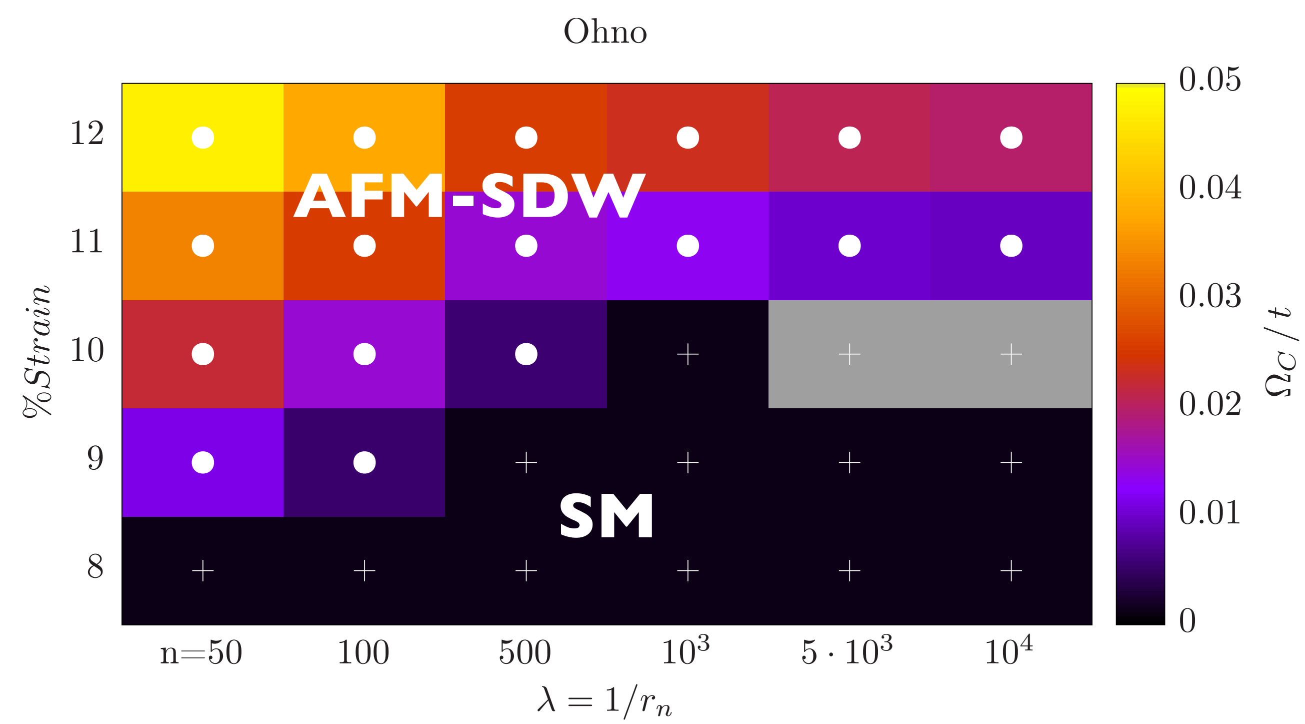
- **longer-ranged bare interactions:**
  - strain: $r \to (1+\eta)r$
    $t \to t_0 e^{-3.37\eta}$

cRPA

Ohno interaction profile

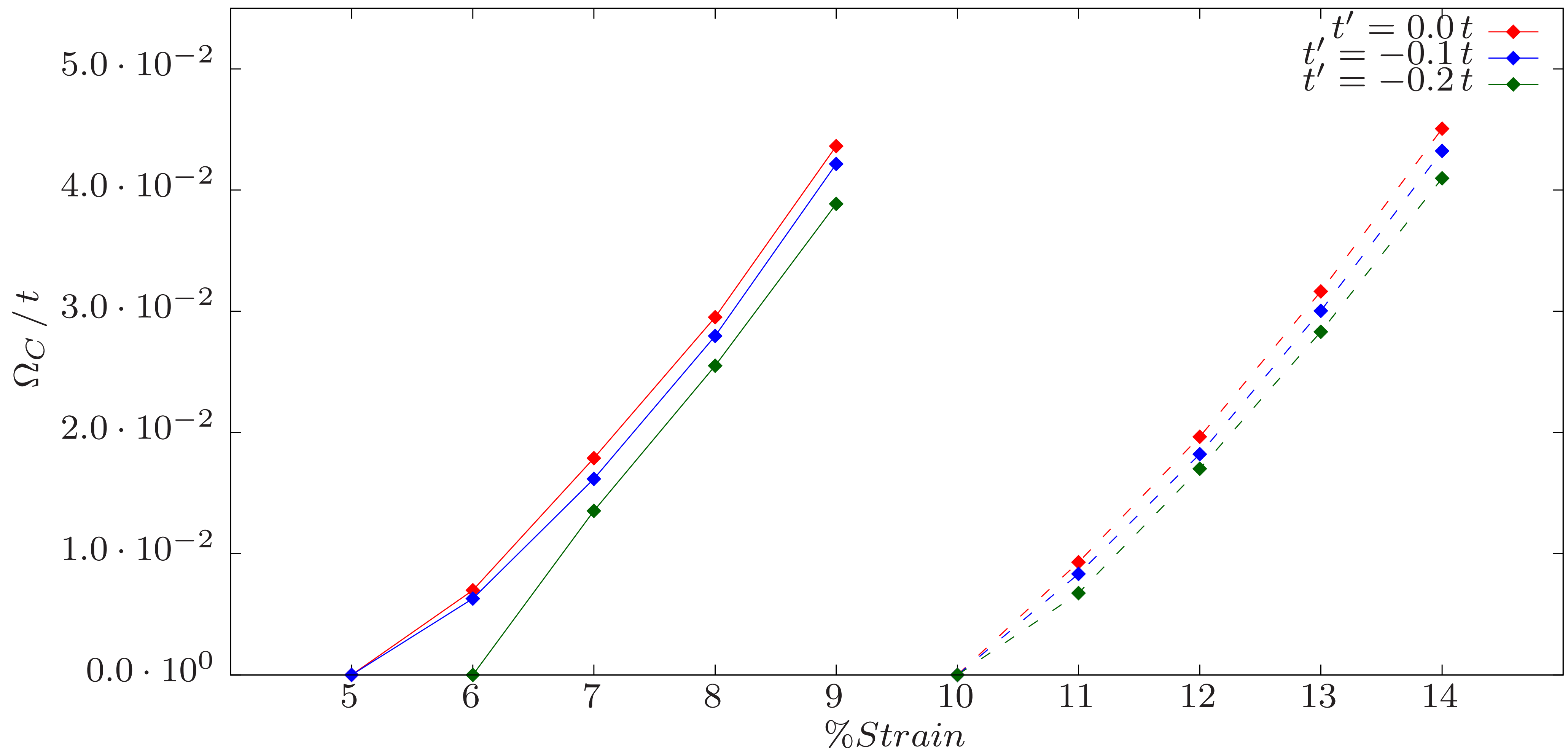
$$V(r_{ij},\epsilon) = \frac{U}{\sqrt{1+\left(\epsilon\,\frac{U}{e^2} r_{ij}\right)^2}}$$





Interaction-induced **AFM instablity** under strain

$$H = H_0 + H_{\mathrm{int}} \quad \& \text{ strain}$$



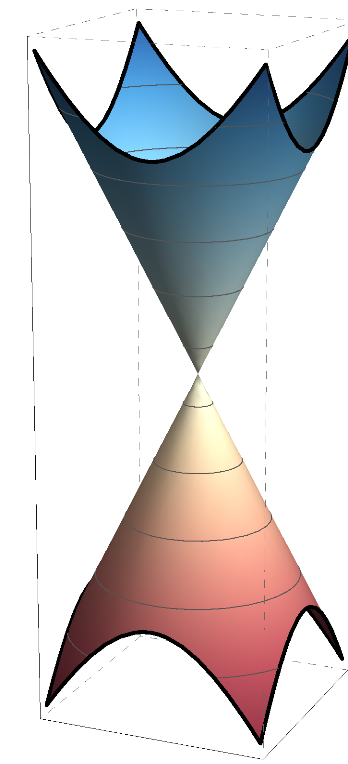
- t-t'-Coulomb model with ab initio parameters including effects of strain
- SM phase for zero strain (in agreement with experiment and QMC)
- finite amount of strain drives system into AFM regime
- can explore ab initio interaction profiles inaccessible for QMC (t' \neq 0 and larger non-local i.a. terms)

(II) **Dirac fermions** and **critical phenomena**

with Bernhard Ihrig, Nikolai Zerf, Luminita Mihaila and Igor Herbut

Effective theory for fermions on the honeycomb lattice

$$H_0 = -t \sum_{\vec{R},i} \left[u^\dagger(\vec{R}) v(\vec{R} + \vec{\delta}_i) + \text{h.c.} \right]$$



- energy: linear & isotropic near ***K, K'***
- retain only Fourier components around ***K, K'***
- action at low-energies corresponding to H_0:

$$S = \int_0^{1/T} d\tau d\vec{x} \sum_{\sigma=\pm 1} \bar{\psi}_\sigma(\vec{x},\tau) \gamma_\mu \partial_\mu \psi_\sigma(\vec{x},\tau)$$

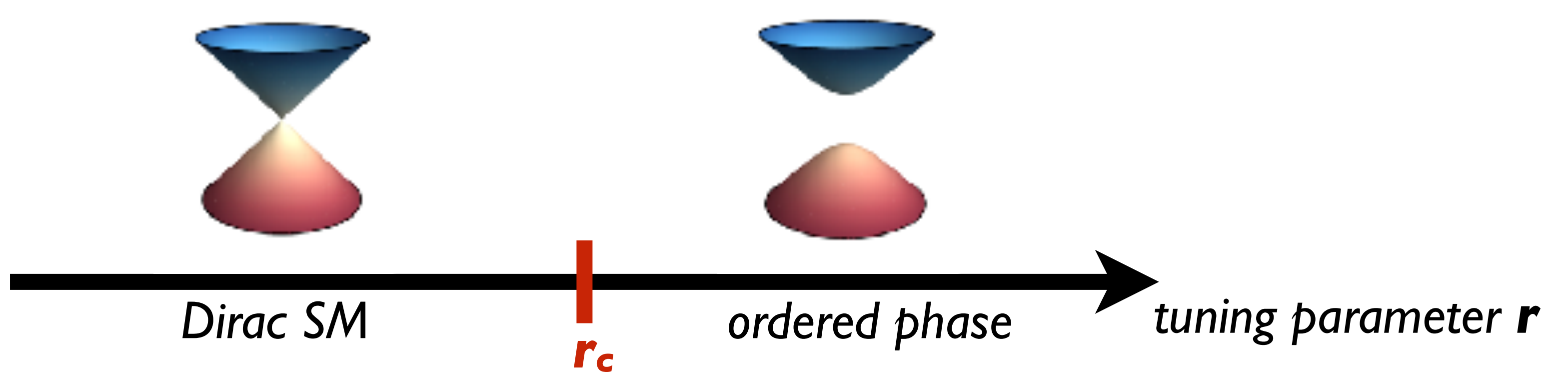
- with 8-component spinor:

$$\psi_\sigma^\dagger(\vec{x},\tau) = T \sum_{\omega_n} \int^\Lambda \frac{d\vec{q}}{(2\pi a)^2} e^{i\omega_n + i\vec{q}\cdot\vec{x}} \left[u^\dagger(\vec{K}+\vec{q},\omega_n), v^\dagger(\vec{K}+\vec{q},\omega_n), u^\dagger(-\vec{K}+\vec{q},\omega_n), v^\dagger(-\vec{K}+\vec{q},\omega_n) \right]$$

- and γ matrices: $\gamma_0 = I_2 \otimes \sigma_z \,, \quad \gamma_1 = \sigma_z \otimes \sigma_y \,, \quad \gamma_2 = I_2 \otimes \sigma_x$
- generalize to arbitrary number of pairs of Dirac cones N (for spin-1/2: N=2)

Dirac **fermions** and **critical phenomena**

- emergence of **Dirac, Weyl & Majorana** quasi-particle excitations in many materials
- **gapless Dirac fermions** in 2+1 dimensions have **quantum critical points**
    - *interacting electrons in graphene*: charge order/antiferromagnetic order
    - *3D topological insulators*: surface states with *emergent* SUSY at superconducting QCP



➡ (2+1)D **fermionic universality classes**

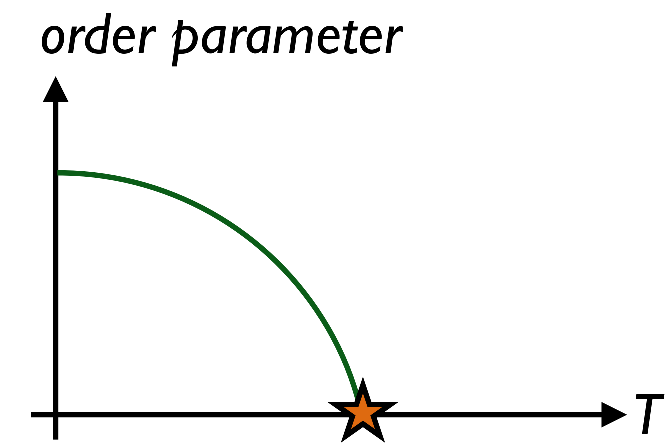
- *What are their critical exponents?*

Recap: **Phase transitions** and **critical phenomena**

- near critical point of continuous phase transition: **universality**
- order parameter **correlation function** for large *r*:

$$G(\vec{r},t) = \langle (m(\vec{r}) - m) m(\vec{0}) - m) \rangle \propto \frac{e^{-r/\xi(t)}}{r^{d-2+\eta}}$$

- with **correlation length**: $\xi(t) \propto |t|^{-\nu}$



- **3D Ising universality class** from complementary methods:

Method	ν	η	
conformal bootstrap	0.629971(4)	0.036298(2)	Kos *et al.* (2016)
Monte Carlo	0.63002(10)	0.03627(10)	Hasenbusch (2010)
pRG, 4-ε, 6th order	0.6292(5)	0.0362(2)	Panzer & Kompaniets (2017)
functional RGs, DE	0.630(5)	0.034(5)	Litim & Zappala (2010)

✓ fantastic agreement across complementary methods!

✦ **gapless Dirac fermions *not* in Ising/O(N) universality classes!**

Effective theory for phase transitions in **Dirac** systems

- described by simple ***continuum*** field theory in $D = 2{+}1$ dimensions Herbut (2006)

  - ***Gross-Neveu model:*** $$\mathcal{L}_{\rm GN} = \bar{\psi}_i \gamma_\mu \partial_\mu \psi_i + g(\bar{\psi}_i \psi_i)^2$$

    - simplest *fermionic theory* with *critical point* (quasi-relativistic, no Fermi surface,…)
    - perturbative RG to 4th order evaluated in ***D* = 2 + ε** Gracey, Luthe & Schroeder (2016)
    - example: **charge density wave** transition of **Dirac electrons** in graphene
    - *bosonized version* of model…

  - ***Gross-Neveu-Yukawa model:*** $$\mathcal{L}_{\rm GNY} = \bar{\psi}_i(\gamma_\mu \partial_\mu + \sqrt{y}\phi)\psi + \frac{1}{2}\phi(m^2 - \partial_\mu^2)\phi + \lambda\phi^4$$

    - perturbatively renormalizable in ***D* = 4 - ε**

✦ both models have **critical point** in **2 < D < 4** and lie in **same universality class**

➡ **Gross-Neveu universality**

Gross-Neveu universality classes

- Gross-Neveu model for **8-component spinor**

- **critical exponents** until **~ 2015:**

Method	$1/\nu$	η_B	η_F	
2+ε, 3rd order	0.764	0.602	0.081	Gracey (1994)
4-ε, 2nd order	1.055	0.695	0.065	Rosenstein *et al.* (1994)
quantum Monte Carlo	1.20(1)	0.62(1)	0.38(1)	Chandrasekharan & Li (2013)
functional RG, DE	0.982	0.760	0.032	Janssen & Herbut (2014)
conformal bootstrap	-	-	-	

- **no** satisfactory **agreement** has been achieved for **fermionic universality classes**!

Fermionic universality classes - **recent developments**

- *precision determination* of Gross-Neveu universality class seems *now within reach*:

  - ***quantum Monte Carlo methods:***
    - microscopic lattice models with 2nd order phase transition in GN universality class
    - sign-problem free formulations

    Chandrasekharan & Li (2013)
    Wang, Corboz & Troyer (2014)
    Li, Jiang & Yao (2015)
    Hesselmann & Wessel (2016)
    Huffmann & Chandrasekharan (2017)
    Li, Vaezi, Mendl, Yao (2017)

  - ***conformal bootstrap:***
    - unprecedented precision for O(N) models
    - now extended to fermionic systems

    Bashkihrov (2013)
    Iliesiu et al. (2016, 2017)

  - ***renormalization group approaches:***
    - progress in application of non-perturbative FRG methods (GRK!)

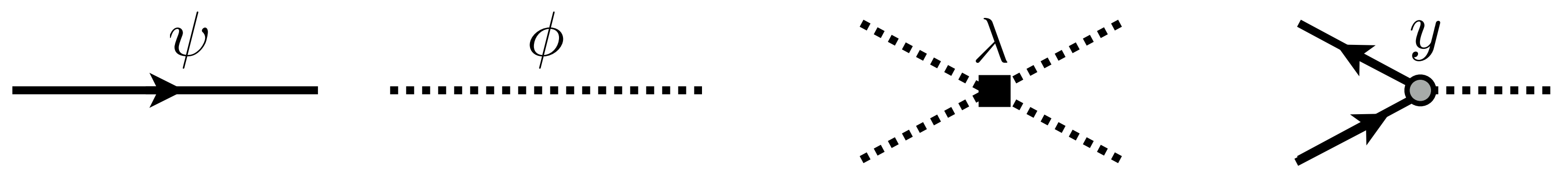
    Vacca & Zambelli (2015)
    Borchardt & Knorr (2016)
    Gies, Hellwig, Wipf, Zanusso (2017)
    Feldmann, Wipf, Zambelli (2017)
    Knorr (2016,2018)

    - *higher-loop calculations adapted from high-energy physics up to 4-loop order!*

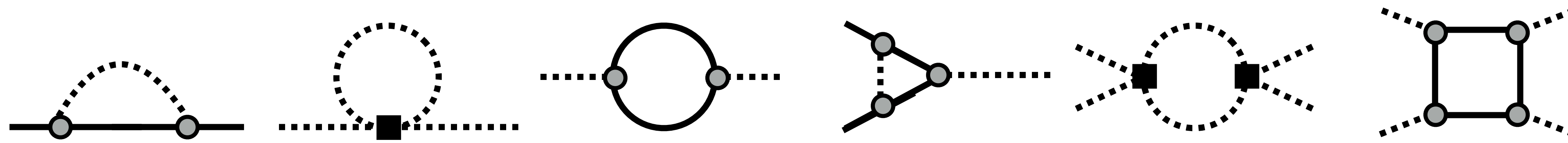
    Gracey, Luthe & Schroder (2016)
    Mihaila, Zerf, Marquard, Ihrig, Herbut , MMS (2017,2018)

Renormalization group constants — **tool chain**

- evaluate renormalization group constants Z_i for GNY model up to 4-loop order
- tree level:



- 1 loop:



…

- 4 loops: *in total **31,671 diagrams!***

  ‣ **use tool chain developed for relativistic high-energy physics:**

QGRAF ‣ *insert Lagrangian - generates complete set of diagrams with symmetry factors*

→ **Q2E** ‣ *declare mass scales and Feyman rules*

→ **EXP** ‣ *reduce to one-scale integrals by asymptotic expansion*

→ **FORM** ‣ *reduce integrals to 19 known master-integrals using* **Crusher**

Quantum critical behavior of massless Dirac electrons

- obtain **critical exponents** in $D = 4 - \varepsilon$, e.g. for $N = 8$:

$$\frac{1}{\nu} \approx 2 - 0.9524\epsilon + 0.007225\epsilon^2 - 0.09487\epsilon^3 - 0.01265\epsilon^4 \,,$$
$$\eta_\phi \approx 0.5714\epsilon + 0.1236\epsilon^2 - 0.02789\epsilon^3 + 0.1491\epsilon^4 \,,$$
$$\eta_\psi \approx 0.07143\epsilon - 0.006708\epsilon^2 - 0.02434\epsilon^3 + 0.01758\epsilon^4 \,.$$

✓ results available for all N and coupling to Ising, XY and Heisenberg OP

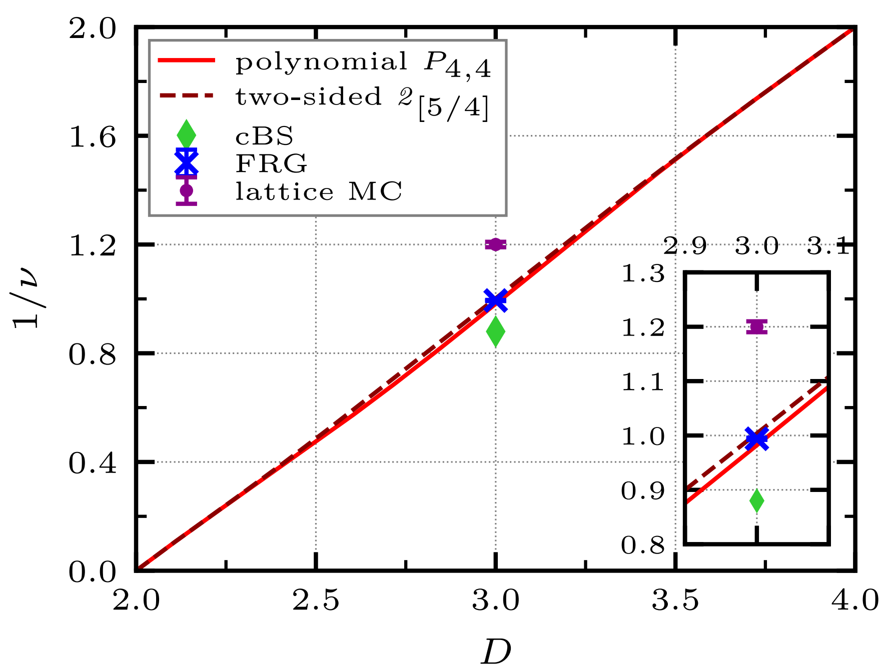
✓ compatible with all previously known results (GNY to order ε^2, ϕ^4 to order ε^4, $1/N^2$)

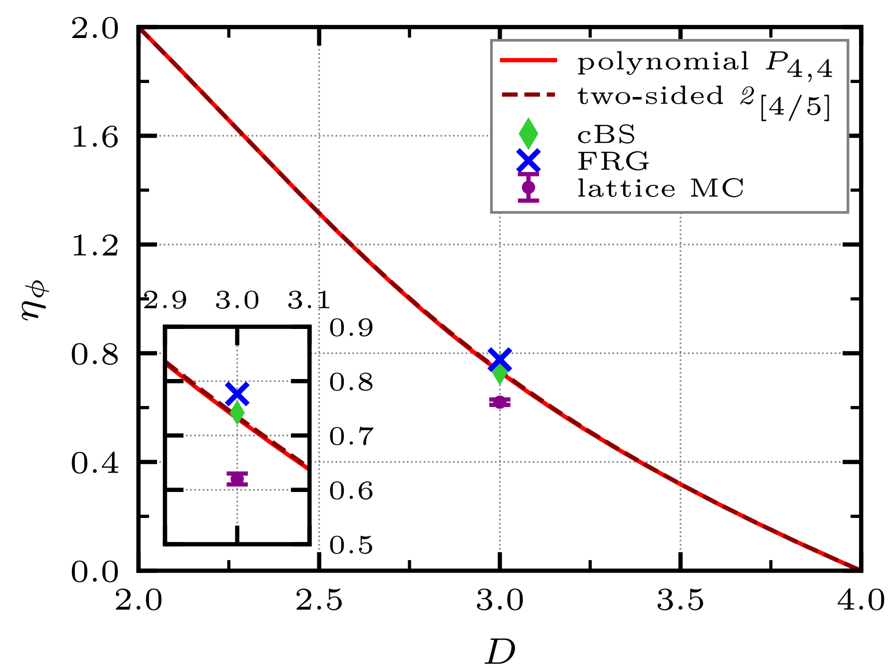
- perturbative expansion is ***asymptotic series*** - cannot simply set $\varepsilon = 1$
    - *employ Padé approximants*

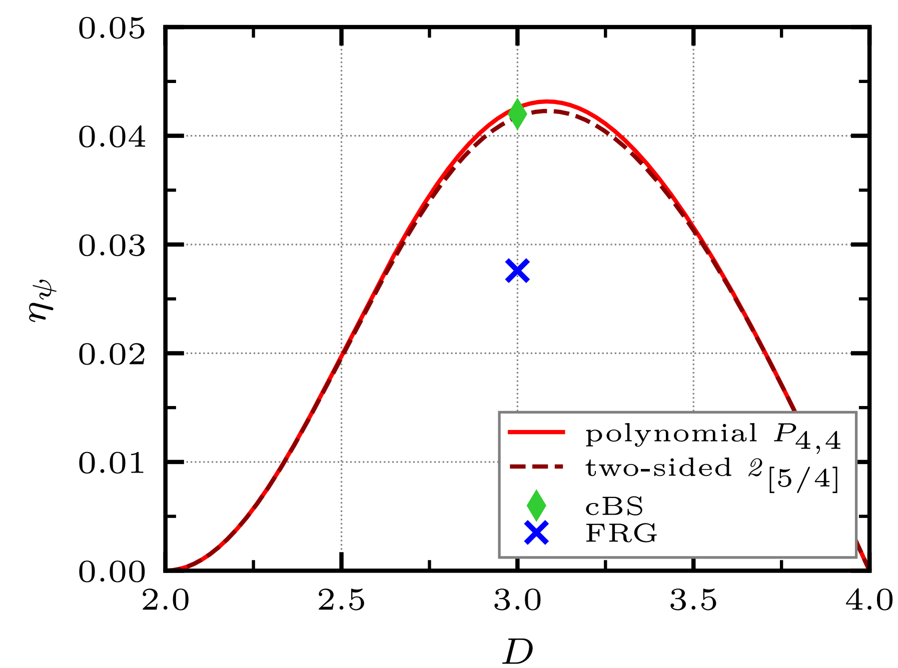
Quantum critical behavior of massless Dirac electrons

- use with $D = 2 + \varepsilon$ expansion to order ε^4 for estimates of critical exponents at $D = 2 + 1$

  - ***employ polynomial interpolation and 2-sided Padé approximants for N = 8:***







  - currently: play around with Borel transfromation/sums, conformal mapping,…

  - emergent SUSY for N = 1:

$N = 1$	ν^{-1}	η_ϕ	η_ψ
Sec. **V**	1.415(12)	0.1673(27)	0.1673(27)
conformal bootstrap[10]	*1.418*	0.164	0.164
functional RG[25]	1.395	0.167	0.167

  - emergent SUSY for N = 2 and complex OP:

	$1/\nu$	η_ϕ	η_ψ
this work, $P_{[2/2]}$	1.128	1/3	1/3
this work, $P_{[3/1]}$	1.130	1/3	1/3
conformal bootstrap[88]	1.090	1/3	1/3
QMC	1.15(6)	0.32(2)	0.34(5)
FRG	1.166	1 / 3	1 / 3

— Conclusion & Outlook —

Summary & **conclusions**

- **Quantum critical behavior of Dirac fermions:**
  - *analytical expressions for arbitrary N and other order parameters to order* ε^4 $(D = 4 - \varepsilon)$
  - ***excellent agreement*** with ***conformal bootstrap*** for anomalous dimensions for $N = 8$
  - ***excellent agreement*** for SUSY cases with $N = 1$ (Ising OP) and $N = 2$ (complex OP)
  - good chance to settle ***GN critical exponents*** across different methods, soon!
  - serious ***mismatch with current QMC results*** — what's up there? anyone?

Mihaila, Zerf, Ihrig, Herbut, MMS (2017)
Zerf, Mihaila, Marquard, Herbut, MMS (2017)
… to appear soon (2018)

- **Many-body instabilities of honeycomb electrons:**
  - *unbiased determination of* ***leading ordering*** *tendency for arbitrary interaction profiles*
  - *Coulomb-tail* does not lead to other instabilities than ***U-driven AF order***
  - unstrained model ***compatible with SM*** *behavior and* ***QMC***
  - uniform strain helps to get to **AF order**

Sánchez de la Peña, Lichtenstein, Honerkamp, Scherer (2017)