Phase transitions and critical behavior in 2D Dirac materials

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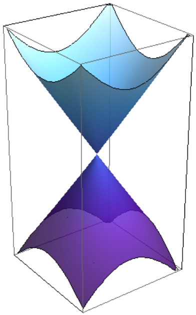
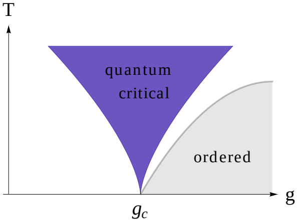
Outline

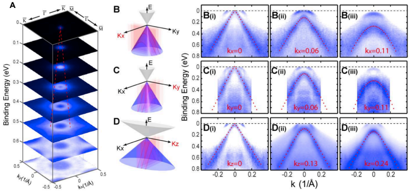
- 2D Dirac materials
  - From hopping electrons to Dirac fermions
  - Ordered phases/Chiral symmetry breaking
- Multicriticality between density waves
  with Michael Scherer, Lukas Janssen and Igor Herbut
- Kekulé order and fermion-induced quantum criticality
  with Michael Scherer and Igor Herbut





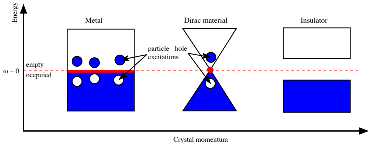
Dirac Materials

- Graphene, Silicene and Germanene
- 3D Dirac materials, artificial graphenes, ...



Z.K.Liu *et al*
Science 343 (2014)

- Universal properties as consequence of Dirac spectrum

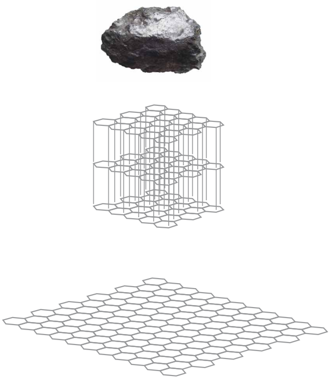


T.O.Wehling *et al*
Adv. Phys. 76 (2014)

- Semimetal - stable against weak interactions

Graphene

- In 2004 K. S. Novoselov and A. K. Geim fabricated free-standing graphene
- 2D material
- 1 layer of graphite
- Hexagonal lattice of carbon atoms

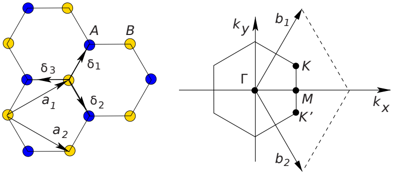


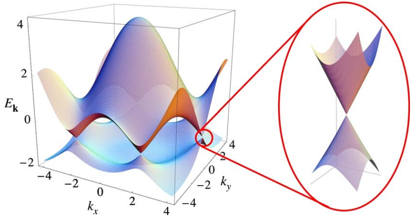
Free electrons in graphene

- Hopping of free electrons:

$$H = -t \sum_{\langle i,j \rangle, s} c^\dagger_{i,A,s} c_{j,B,s} + \text{h.c.}$$

- *ab initio* $t \approx 2.8$ eV



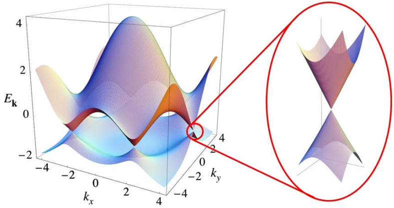


- Energy bands show semimetallic behavior
- Half filling: at $E = 0$ bands touch at Dirac points $\mathbf{K}, \mathbf{K}'$
- Linear and isotropic energy spectrum at $\mathbf{K}, \mathbf{K}'$

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

From hopping to Dirac electrons

- Approximation at low energies: Retain only modes near $\mathbf{K}, \mathbf{K}'$



- Low energy effective action

$$S_F = \int_0^{1/T} d\tau d^{D-1}x \ \bar{\Psi}\gamma_\mu \partial_\mu \Psi$$

- with 8-component spinor $\Psi = (\Psi_\uparrow, \Psi_\downarrow)^T$ and $\bar{\Psi} = \Psi^\dagger \gamma_0$

$$\Psi_s^\dagger(x,\tau) = \int_q^\Lambda e^{i\omega_n\tau + iq\cdot x}\left[c_{A,s}^\dagger(K+q,\omega_n), c_{B,s}^\dagger(K+q,\omega_n), c_{A,s}^\dagger(K'+q,\omega_n), c_{B,s}^\dagger(K'+q,\omega_n)\right]$$

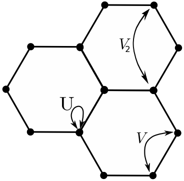
- and γ matrices

$$\gamma_0 = \mathbb{1}_2 \otimes \sigma_z, \quad \gamma_1 = \sigma_z \otimes \sigma_y, \quad \gamma_2 = \mathbb{1}_2 \otimes \sigma_x$$

Interactions and phase transitions

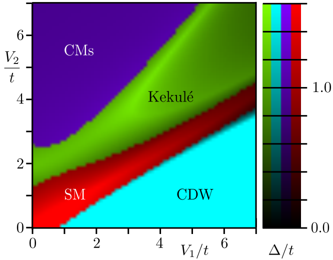
- Repulsive Coulomb interactions ($n_{i,s} = c^\dagger_{i,A/B,s} c_{i,A/B,s}$)

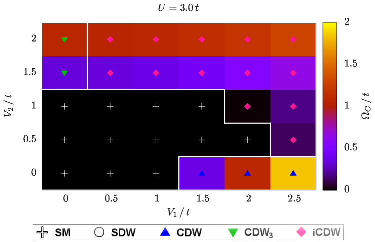
$$H_{int} = U \sum_i n_{i,\uparrow} n_{i,\downarrow} + V \sum_{\langle i,j \rangle, s, s'} n_{i,s} n_{j,s'} + V_2 \sum_{\langle\langle i,j \rangle\rangle, s, s'} n_{i,s} n_{j,s'} + \dots$$



- Long-ranged tail unscreened, but marginally irrelevant
- Short-ranged interactions can induce quantum phase transition, but critical strength needed
- Different orders depending on interaction profile

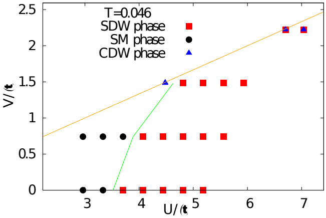
Quantum phase diagrams





ED: García-Martínez et al PRB 88 (2013)

FRG: Peña et al arXiv:1606.01124



HMC: Buividovich et al

PoS (LATTICE2016) 244

- Semimetallic phase (SM) for small interactions
- Spin Density Wave for large U
- Charge Density Wave for large V
- Often Kekulé order for V∼V_2

Chiral symmetry breaking

- Effective low-energy theory $S_F = \int d^D x \; \bar{\Psi}\gamma_\mu \partial_\mu \Psi$
- Describe interaction-induced phase transitions with chiral symmetry breaking
- Gross-Neveu-Yukawa theory $S = S_F + S_B + S_Y$
- S_B: Order parameter fields
- Fermion and boson coupling

$$S_Y = \int d\tau d^{D-1} x g_i \varphi_i \bar{\Psi} M_i \Psi$$

$$M_{CDW} = \mathbb{1} \quad M_{SDW} = \vec{\sigma} \quad M_{Kekule} = \gamma_3, \gamma_5$$

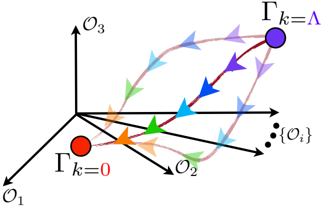
- E.g. CDW: $\bar{\Psi}\Psi \sim \sum_{k,s} c^\dagger_{A,k,s} c_{A,k,s} - c^\dagger_{B,k,s} c_{B,k,s}$
  $\rightarrow$ Difference of sublattice densities
- Generalize number of Dirac points N_f (graphene $N_f = 2$)

FRG and truncation

- Full theory in effective action $\Gamma(g_1, g_2, \dots)$
- Integrate out dof's successively - Systematic implementation by (additive) regulator R_k
- Flow equation   Wetterich PLB 301 (1993)

$$\partial_t \Gamma = \frac{1}{2} \mathrm{STr}(\Gamma_k^{(2)} + R_k)^{-1} \partial_t R_k$$

with full propagator $(\Gamma_k^{(2)} + R_k)^{-1}$



L. Fister

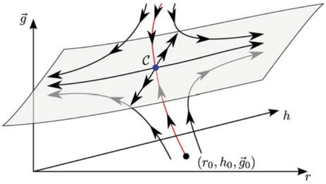
- Truncation

$$\Gamma_k = \int d^D x \Big(Z_{\Psi,k} \bar{\Psi} \gamma_\mu \partial_\mu \Psi - \frac{1}{2} Z_{\varphi_i,k} \varphi_i \partial_\mu^2 \varphi_i + \bar{g}_{i,k} \varphi_i \bar{\Psi} M_i \Psi + U_k(\varphi_i) \Big)$$

- Differential equations for couplings (β functions) encode scale evolution
- Non-perturbative regime $D = 2 + 1$, $N_f = 2$ directly accessible

Fixed points and critical behavior

- Fixed points ($\partial_k g_i = \beta_{g_i} = 0$)
  $\rightarrow$ scale-free points
  $\rightarrow$ 2nd order phase transition
- Scaling properties given by critical exponents



P. Kopietz, Springer Verlag 2010

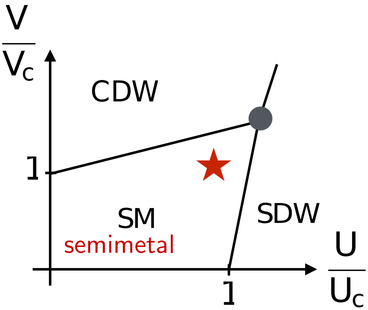
- Extract critical exponents from linearized β functions at FP

$$\beta_{g_i}(\{g_n\}) = \sum_j \frac{\partial \beta_{g_i}}{\partial g_j}\bigg|_{g_n = g_n^*} (g_j - g_j^*)$$

- Sign of negative eigenvalues ($\pm$) determines (ir)relevant directions
- Relevant directions determine stability: Is FP approachable ?
  - Number of tuning parameters = number of relevant directions for stable FP
- No such FP $\rightarrow$ 1st order phase transition

SDW and CDW: competition and multicriticality

Phase diagram with U and V

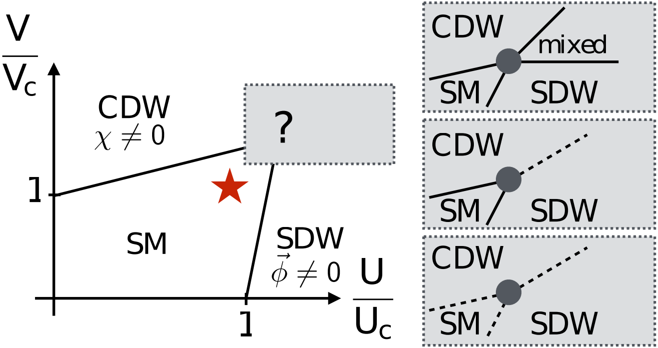


	Graphene		Graphite	
	Bare	cRPA	Bare	cRPA
$U_{00}^{A\,\mathrm{or}\,B}$ (eV)	17.0	9.3	17.5, 17.7	8.0, 8.1
U_{01} (eV)	8.5	5.5	8.6	3.9
$U_{02}^{A\,\mathrm{or}\,B}$ (eV)	5.4	4.1	5.4, 5.4	2.4, 2.4
U_{03} (eV)	4.7	3.6	4.7	1.9

- Experiment: graphene is SM
- But close to phase transition:
  - Compare critical interactions with e.g. cRPA
    Wehling *et al* PRL 106 (2011)
  - Mild increase of interaction leads to phase transition
    Ulybyshev *et al* PRL 111 (2013)
    Smith, Smekal PRB 89 (2014)
  - Sizable charge-density and spin-current correlations
    Golor, Wessel PRB 92 (2015)
  - Isotropic strain of $\sim 15\%$ can induce transition
    H.-K Tang *et al* PRL 115 (2015)

- Separate transitions: chiral Ising/Heisenberg universality class
  Janssen, Herbut PRB 89 (2014), Vacca, Zambelli PRD 91 (2015), Parisen et al PRB 91 (2015), Otsuka et al, PRX 6 (2016), Knorr PRB 94 (2016),...

Multicritical behavior in graphene



- Graphene parameters close to multicritical point
- Competition of order parameters
- Structure at MCP? Critical exponents?

Coupled order parameter fields

- CDW field $\chi = \left\langle \bar{\Psi}\Psi \right\rangle$ and SDW field $\vec{\phi} = \langle \Psi\vec{\sigma}\Psi \rangle$
- Symmetry of CDW and SDW fields is $\mathbb{Z}_2$ and $O(3)$
- Two Yukawa terms

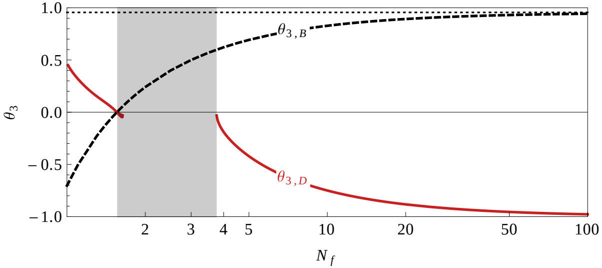
$$S_Y = \int d^D x \left[g_\chi \chi \bar{\Psi}\Psi + g_\phi \vec{\phi} \cdot \bar{\Psi}\vec{\sigma}\Psi \right]$$

- Coupling between different oder parameter fields

$$S_B = \int d^D x \Big[\frac{1}{2}\chi(-\partial_\mu^2 + m_\chi^2)\chi + \frac{1}{2}\vec{\phi} \cdot (-\partial_\mu^2 + m_\phi^2)\vec{\phi} \\ + \frac{\lambda_\chi}{8}\chi^4 + \frac{\lambda_\phi}{8}\big(\vec{\phi} \cdot \vec{\phi}\big)^2 + \frac{\lambda_{\chi\phi}}{4}\chi^2\vec{\phi}^2 + \ldots \Big]$$

Fixed point structure

- 2 tuning parameters, i.e. stable FP can have 2 relevant directions
- Sign of third critical exponent determines stability

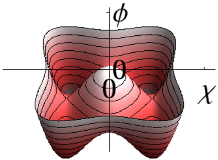


- Two candidates for stable FP
  - Chiral Heisenberg + Ising for small N_f
  - New universality from coupled FP for large N_f
- Mid-size N_f: no stable FP $\rightarrow$ 1st order transition

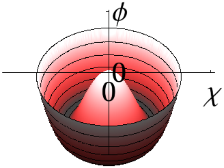
Multicritical behavior at stable FP

- Determine phase structure from effective potential
- Positions of minima determined by $\Delta = \lambda_\chi \lambda_\phi - \lambda_{\chi\phi}^2$

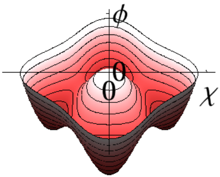
$\Delta > 0$



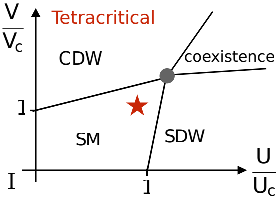
$\Delta = 0$



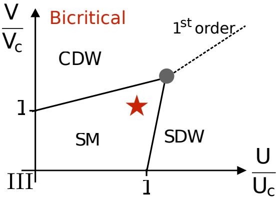
$\Delta < 0$



$\Delta > 0$

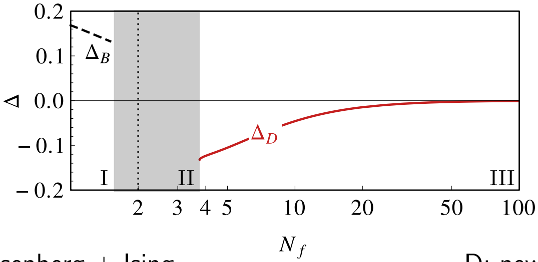


$\Delta < 0$



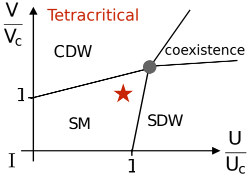
Phase diagram as function of N_f

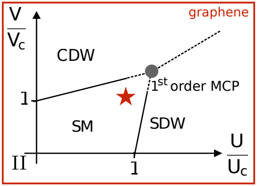
- $\Delta = \lambda_\chi \lambda_\phi - \lambda_{\chi\phi}^2$ determines multiciritcal behavior

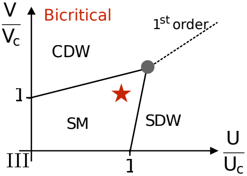


B: chiral Heisenberg + Ising

D: new coupled FP







Kekulé order and fermion-induced criticality

Kekulé Valence Bond Solid

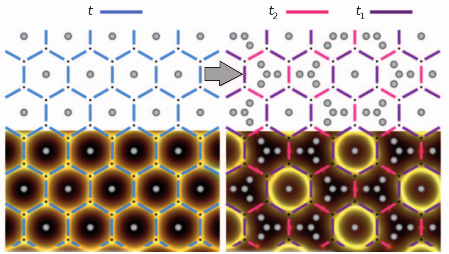
- Bond-dependent nearest-neighbor hopping

$$H_K = -\sum_{i,s,\delta} \Delta t_{i,\delta} c^\dagger_{i,A,s} c_{i+\delta,B,s} + \text{h.c.}$$

- Breaks lattice translation and rotation symmetry $C_6 \to C_3$
- Order can be induced by sufficiently strong
  - electronic interactions $V \sim V_2$

    Hou et al (2007), Weeks/Franz (2010), Roy/Herbut (2010),...
  - Electron-phonon interaction

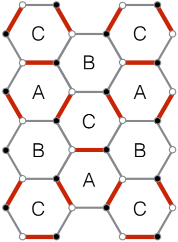
    Nomura et al (2009), Kharitonov (2012), Classen et al (2014),...
- Observed in graphene on Copper substrate and artificial graphene



Gomes et al Nature 483 (2012)

Low energy model for Kekulé order

- Described by complex order parameter $\phi = \phi_1 + i\phi_2$ with $\mathbb{Z}_3$ symmetry



- Dirac fermions $\mathcal{L}_F = \bar{\psi}\gamma_\mu\partial_\mu\psi$
- Coupling between fermions and order parameter fields

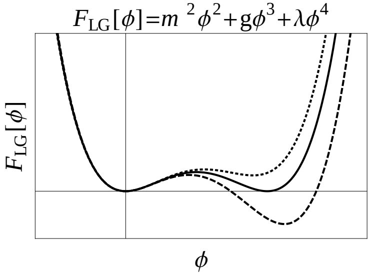
$$\mathcal{L}_Y = ih\bar{\psi}(\phi_1\gamma_3 + \phi_2\gamma_5)\psi$$

- Cubic terms in free energy allowed

$$\mathcal{L}_B = -\phi^*\partial_\mu^2\phi + m^2\,|\phi|^2 + g(\phi^3 + \phi^{*3}) + \lambda\,|\phi|^4 + \dots$$

Landau Criterion and Fermion-Induced QCP

- First order transition due to cubic terms
- Presence of fermion critical mode can change Landau picture $\rightarrow$ Fermion-induced quantum critical point



- RG picture: need stable FP for continuous transition
- Here: 1 tuning parameter, i.e. stable FP would have 1 relevant direction

$$\mathcal{L}_B = -\phi^* \partial_\mu^2 \phi + m^2 |\phi|^2 + g(\phi^3 + \phi^{*3}) + \lambda |\phi|^4 + \dots$$

- At Gaussian FP 2 relevant directions

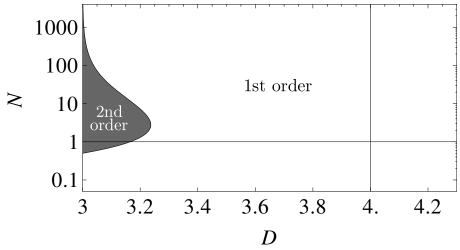
$$[m^2] = 2 \quad [g] = 3 - D/2 \quad [\lambda] = 4 - D$$

- At interacting FP power counting modified

Perturbative RG approaches

- Indeed fermion-induced QCP possible depending on D and N_f
- Corresponding FP has enlarged symmetry $\mathbb{Z}_3 \to U(1)$ (i.e. g=0)
- Large-N_f RG: in 3D critical $N_f = 1/2$ Li et al arXiv:1512.07908
- Expansion around upper critical dimension

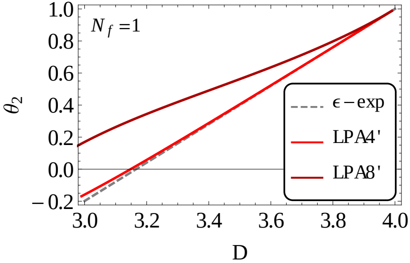
Scherer, Herbut PRB 94 (2016)



- But question is inherently non-perturbative: fluctuations must be strong enough to change sign of canonical dimension of cubic coupling $\to$ employ FRG

Identify wanted fixed point

- Connect to ϵ-expansion: follow FP from D=3 to D=4



LPAn: expansion of effective potential to nth order

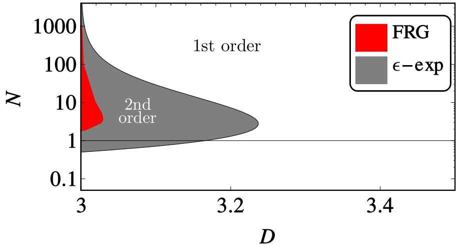
- For $N_f = 1/2$: compare critical exponents to emergent SUSY

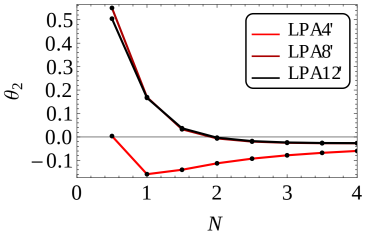
Zerf et al Phys. Rev. B 94 (2016)

method	ν	η_ϕ	η_ψ
ϵ^3	0.985	1/3	1/3
FRG	0.954	0.353	0.323

Fermion-induced QCP from FRG

- Regime of continuous transition severely reduced
- $N_{f,c} \approx 1.9$ in 3D
- Besides threshold effects, reduction comes from higher order couplings
- In D=3 those couplings must be included
- E.g. $g_5(\phi^3 + \phi^{*3})\,|\phi|^2$ is allowed by symmetry and is relevant in $D = 3$ $[g_5] = 5 - 3D/2$

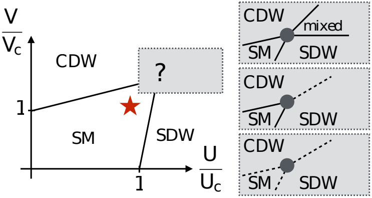




LPAn': expansion of effective potential to nth order + wave function renormalizations

Conclusion

- Material class with emergent Dirac fermions
- New universality classes due to critical Dirac fermion modes
- FRG to access non-perturbative "graphene regime" $D = 2+1$, $N_f = 2$
- Competing orders: SDW and CDW
  - Determine multicritical behavior and phase structure
- Kekulé order
  - 1st order transition rendered continuous for specific D and N_f



Phys. Rev. B 92, 035429 (2015)

Phys. Rev. B 93, 125119 (2016)