Emergent symmetries and lack thereof in quantum critical points in semimetals

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Outline: two study cases

1) Dirac fermions in 2D: graphene

Hubbard model on honeycomb or pi-flux lattice

Mott transition and the "Gross-Neveu universality class"

Emergent Lorentz symmetry at the critical point

(scaling in the magnetic field, and the actual QHE in graphene)

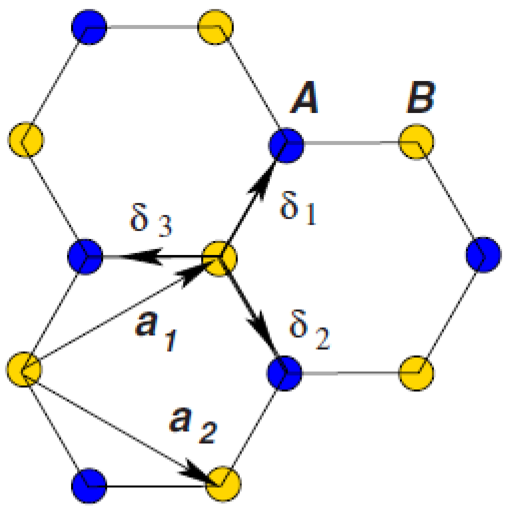
2) Beyond graphene: general ``Dirac systems" ($Z = 2$)

quadratic band touching point in 2D and bilayer graphene

quadratic band touching in 3D: the return of long-range Coulomb

fixed point annihilation, and the hierarchy of scales

1) Graphene (Geim and Novoselov, 2004)



Two triangular sublattices: A and B; one electron per site (half filling)

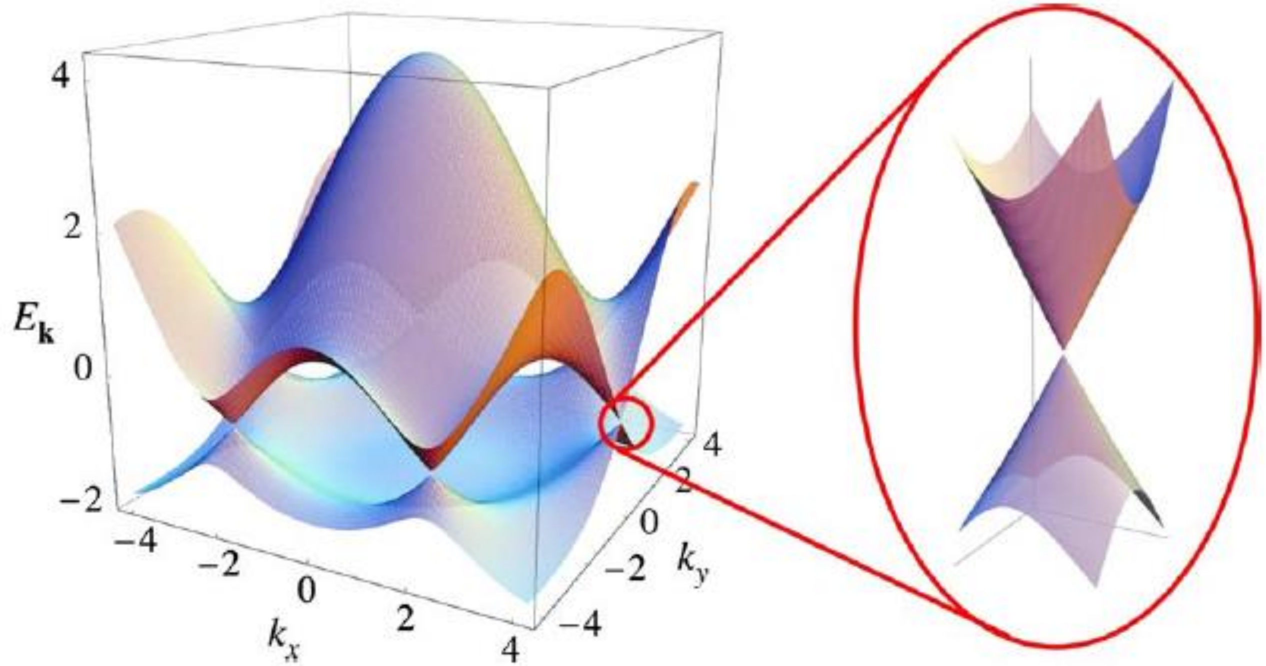
Tight-binding model (t = 2.5 eV):

$$H_0 = -t \sum_{\vec{A}, i, \sigma = \pm 1} u_\sigma^\dagger(\vec{A}) v_\sigma(\vec{A} + \vec{b}_i) + H.c.$$

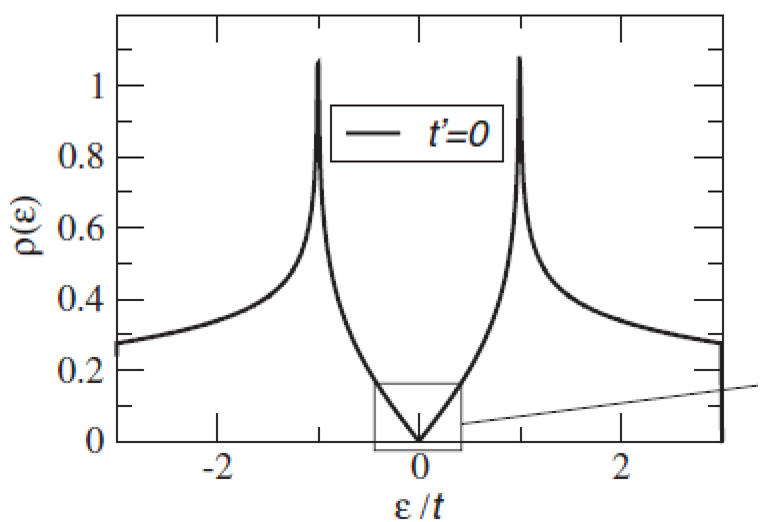
$$E(\vec{k}) = \pm t \left| \sum_i \exp[\vec{k} \cdot \vec{b}_i] \right|$$

The sum is complex => two equations for two variables for zero energy => Dirac points (no Fermi surface)

Particle dispersion:

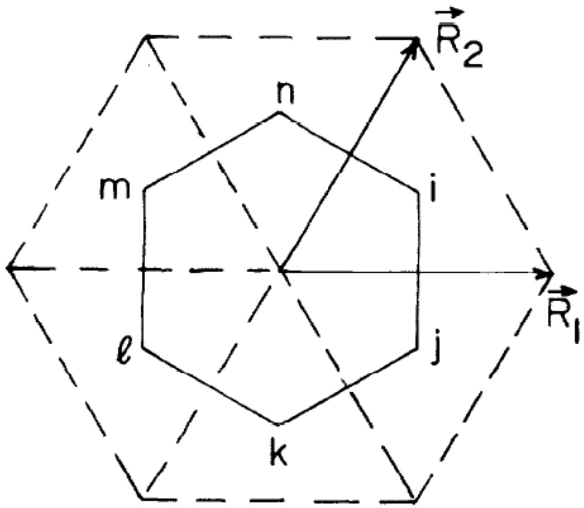


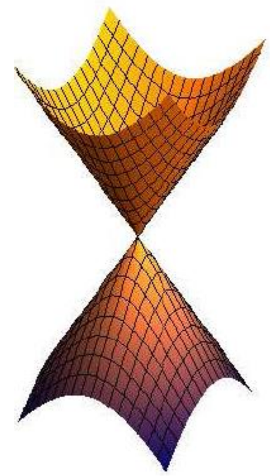
results in the density of states:



which vanishes at half filling!

Brillouin zone:





Two inequivalent Dirac points at :

+K and -K

Dirac fermion: 4 components/spin component

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

“Low - energy” Hamiltonian: $H_0 = i\gamma_0\gamma_i(-i\partial_i - A_i)$ **i=1,2**

$$\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu} \qquad \nu,\, \mu = 0, 1, 2$$

(isotropic, v = c/300 = 1, in our units). Neutrino-like in 2D!

Extended Hubbard model:

$$H = H_0 + H_1$$

with the interaction term, (Hubbard + Coulomb)

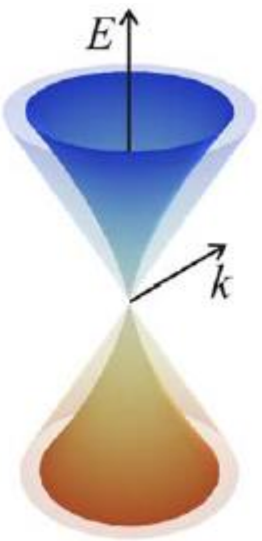
$$H_1 = \sum_{\vec{X},\vec{Y},\sigma,\sigma'} n_\sigma(\vec{X})[\frac{U}{2}\delta_{\vec{X},\vec{Y}} + \frac{e^2(1-\delta_{\vec{X},\vec{Y}})}{4\pi|\vec{X}-\vec{Y}|}]n_{\sigma'}(\vec{Y})$$

Long-range part is not screened, and it may matter even when weak.

Fermi velocity depends on scale:

(Gonzalez, Guinea, Vozmediano, NPB 1994)

$$\rho \frac{\partial}{\partial \rho} v_{eff}(\rho) \;=\; -\beta_v(v_{eff}, e^2_{eff})$$



To the leading order:

$$\rho \frac{\partial}{\partial \rho} \frac{v_{eff}}{v_R} = \frac{1}{16\pi} \frac{e^2}{v_{eff}} + O\left(\frac{e^4}{v^2_{eff}}\right)$$

and the Fermi velocity increases! It goes to where

$$\beta_v(v, e^2) = 0$$

which is at the velocity (in units of velocity of light):

$$\frac{1}{v} \frac{1 - 2v^2 + 4v^4}{(1-v^2)^{3/2}} \, arccos\, v \; + \; \frac{1 - 4v^2}{1 - v^2} = 0 \qquad => \qquad v = 1$$

The ultimate low-energy theory: dimensionally reduced QED3 (matter in 2+1 D + gauge fields in 3+1 D)

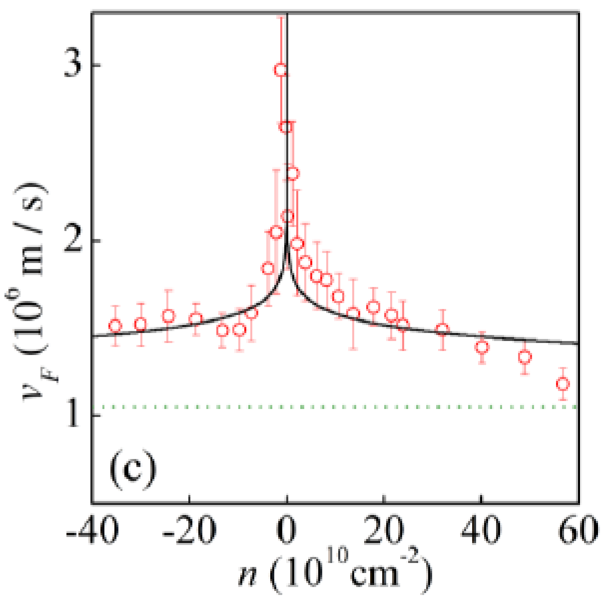
Gauge field propagator:

$$W_{\mu\nu}(\mathbf{x}) = \frac{1}{2}\int \frac{d^3\mathbf{q}}{(2\pi)^3}\frac{e^{i\mathbf{q}x}}{|\mathbf{q}|}\left(\Pi_{\mu\nu}(\mathbf{q}) + \beta\frac{\mathbf{q}_\nu\mathbf{q}_\mu}{\mathbf{q}^2}\right)$$

and the fine structure constant is scale invariant!! Dirac fermions are massless, with a velocity of light.

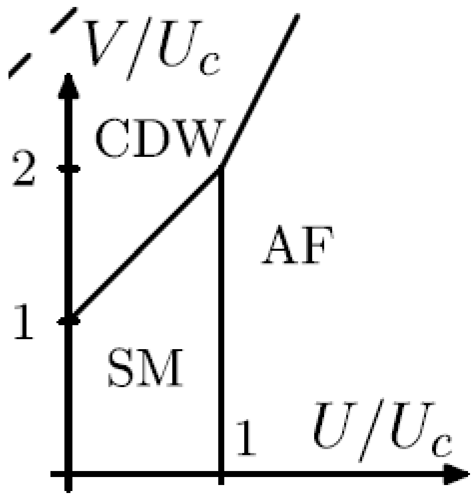
Experiment:

(Ellias , Nature 2011)

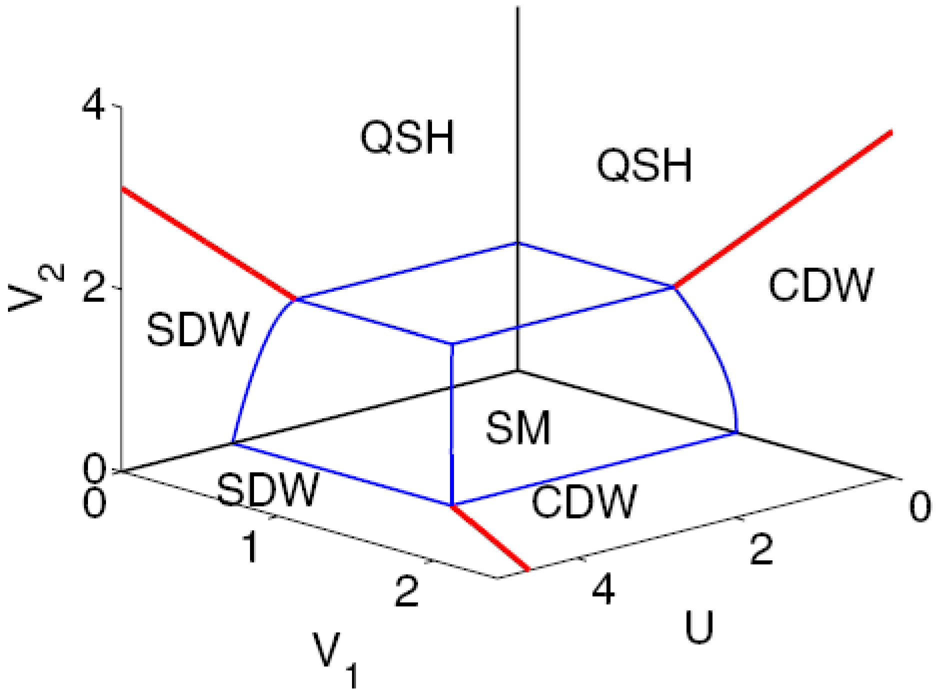


Short-range pieces of Coulomb repulsion:

One may expect:



(IH, PRL 2006)



(Raghu, PRL 2008)

At large interaction some symmetry gets broken.

Gross-Neveu-Yukawa field theory for the Hubbard model

(IH, PRL 2006; IH, Juricic, Roy, PRB 2009; IH, Juricic, Vafek, PRB 2009)

Neel (spin density wave) order parameter:

$$\langle \vec{\phi} \rangle \propto \langle \bar{\Psi}(\vec{\sigma} \otimes \mathbb{1}_4)\Psi \rangle$$

Minimal Ginzburg-Landau-Wilson field theory:

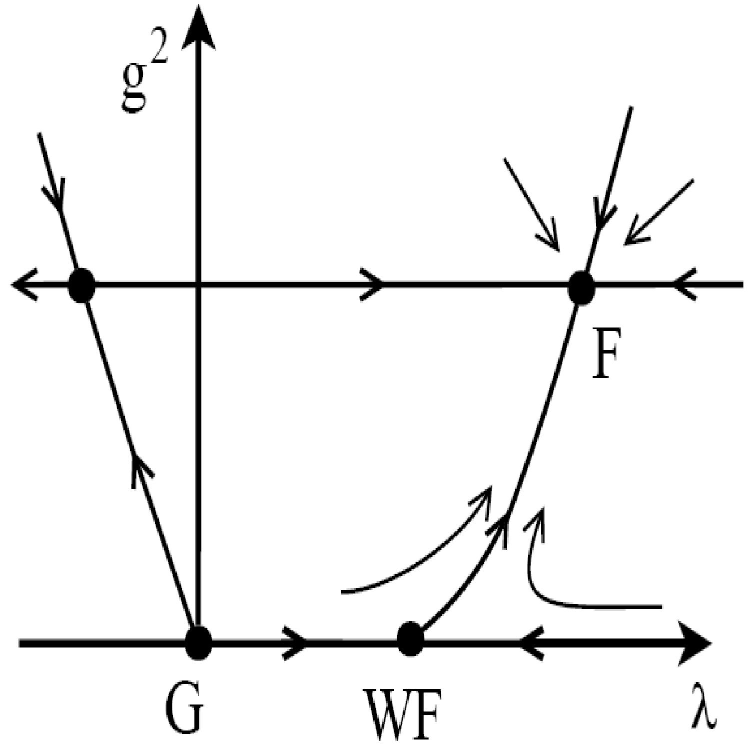
$$\mathcal{S} = \int \mathrm{d}\tau \mathrm{d}^{D-1}\vec{x} \Big[\bar{\Psi}(\mathbb{1}_2 \otimes \gamma_\mu)\partial_\mu \Psi + \frac{1}{2}\phi_a \left(\bar{m}^2 - \partial_\mu^2\right)\phi_a + \bar{\lambda}\left(\phi_a^2\right)^2 + \bar{g}\phi_a \bar{\Psi}(\sigma_a \otimes \mathbb{1}_4)\Psi \Big],$$

(IH, ``A Modern Approach to Critical Phenomena", 2007)

RG flow (epsilon = 3 - dim)

$$\frac{dg_u^2}{d\ln b} = g_u^2(\epsilon - (7-S)g_u^2),$$

$$\frac{d\lambda_u}{d\ln b} = \lambda_u(\epsilon - 8g_u^2) - 4(9+S)\lambda_u^2 + 2g_u^4$$



$S = 0 \ (S = 2)$ **(O(S+1) broken)**

Exponents: $\nu = \frac{1}{2} + \frac{3(5+S)}{(7-S)(9+S)}\epsilon$ $\eta_f = \frac{3}{2(7-S)}\epsilon$ $\eta_b = \frac{4}{7-S}\epsilon$

Long-range "charge": $\frac{de^2}{d\ln b} = -\frac{4}{3}(2\delta_{d,3}+1)e^4$

and marginally irrelevant!

Relativity, again emergent: define a small deviation of velocity

$$\delta_u = 1 - v_{\chi,u} \ll 1$$

it is (the leading) irrelevant perturbation close to d=3 :

$$\frac{d\delta_u}{d\ln b} = \frac{4\epsilon}{S-7}\delta_u$$

(Roy, Juricic, IH, JHEP 2016)

Consequence: universal ratio of specific heats

$$\lim_{T\to 0}\frac{C(t_{\chi,t}\to 0+)}{C(t_{\chi,t}\to 0-)} = 4(1-2^{-d})$$

Direct transition: from gapless (fermions) to gapless (bosons)!

Numerical test: finite size scaling in Hubbard limit, for Neel order parameter, or the gap

$$m = L^{-\beta/\nu} F(L^{1/\nu}(U - U_c))$$

and, near dim=3+1,

$$\frac{\beta}{\nu} = 1 - \frac{\epsilon}{10} + \mathcal{O}\left(\epsilon^2\right)$$

Crossing point and the critical interaction (from magnetization)

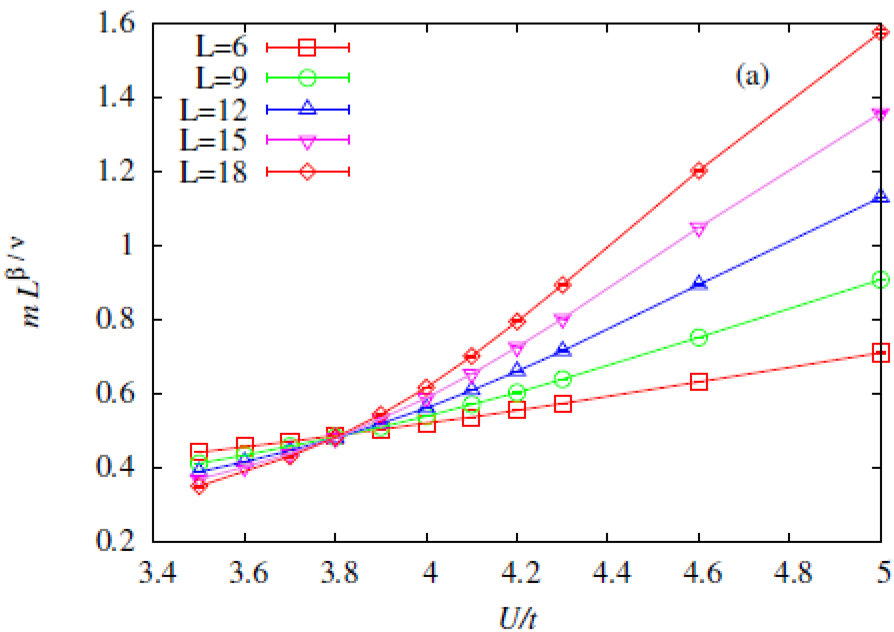


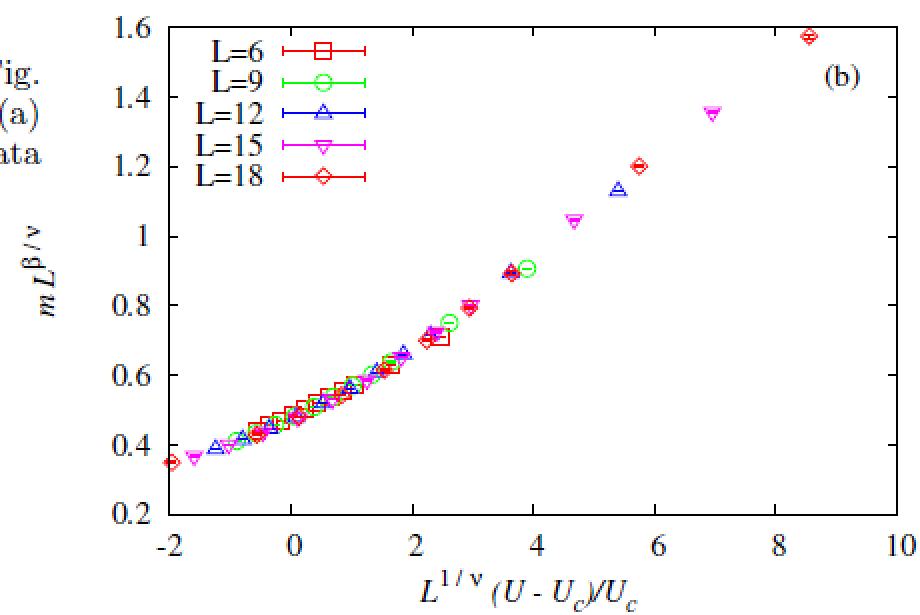
FIG. 5. Data collapse for the magnetization presented in Fig. 3. The exponents are taken for the ϵ-expansion of Ref. 6. (a) The crossing point pins down the value of U_c. (b) The data collapse, using $U_c/t = 3.78$.

This suggests:

U_c = 3.78

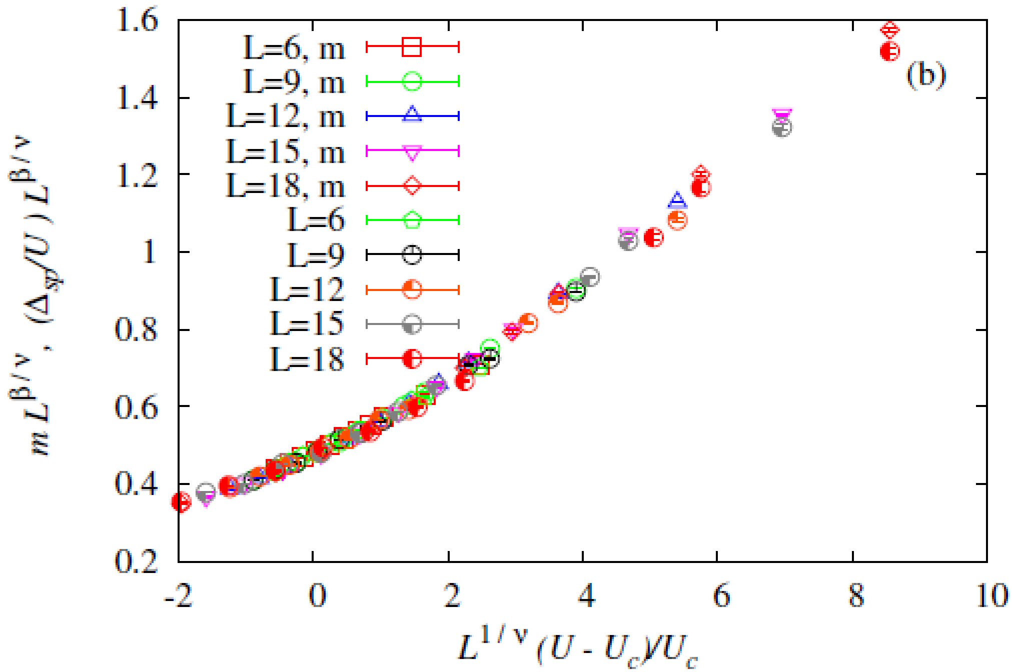
$$\beta/\nu \simeq 0.9$$

$$\nu = \frac{1}{2} + \frac{21}{55}\epsilon + \mathcal{O}\left(\epsilon^2\right)$$



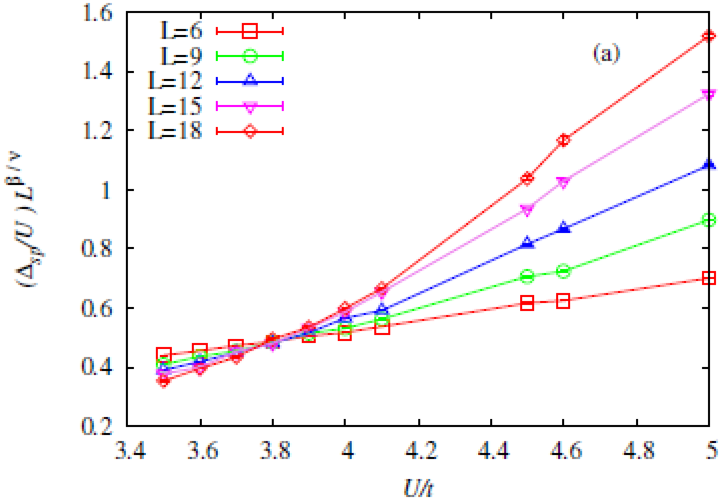
(Assaad and IH, PRX 2013;
Hohenadler et al, PRB 2014;
Parisen Toldin et al, PRB 2015)

Stringent test: single-particle gap (F. Assaad and IH, PRX 2013)



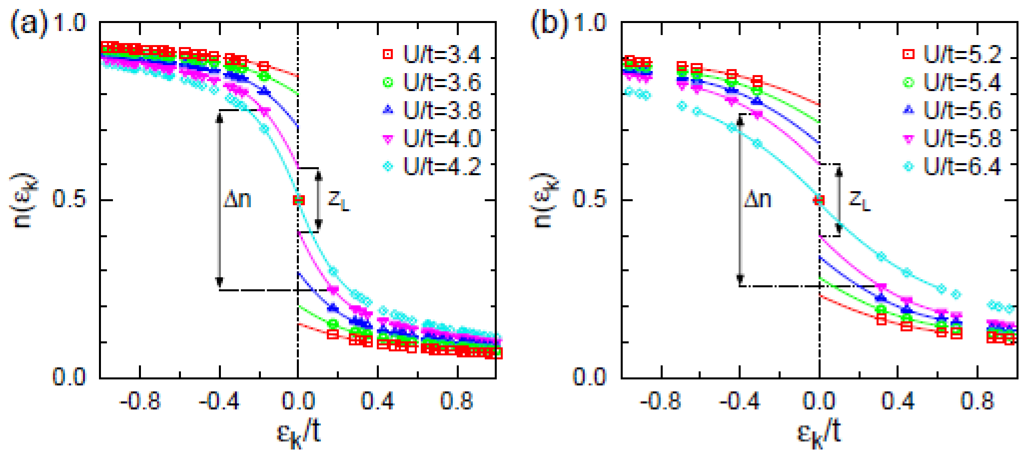
$$\frac{\Delta_{sp}}{U} = L^{-\beta/\nu}\tilde{F}(L^{1/\nu}(U - U_c))$$

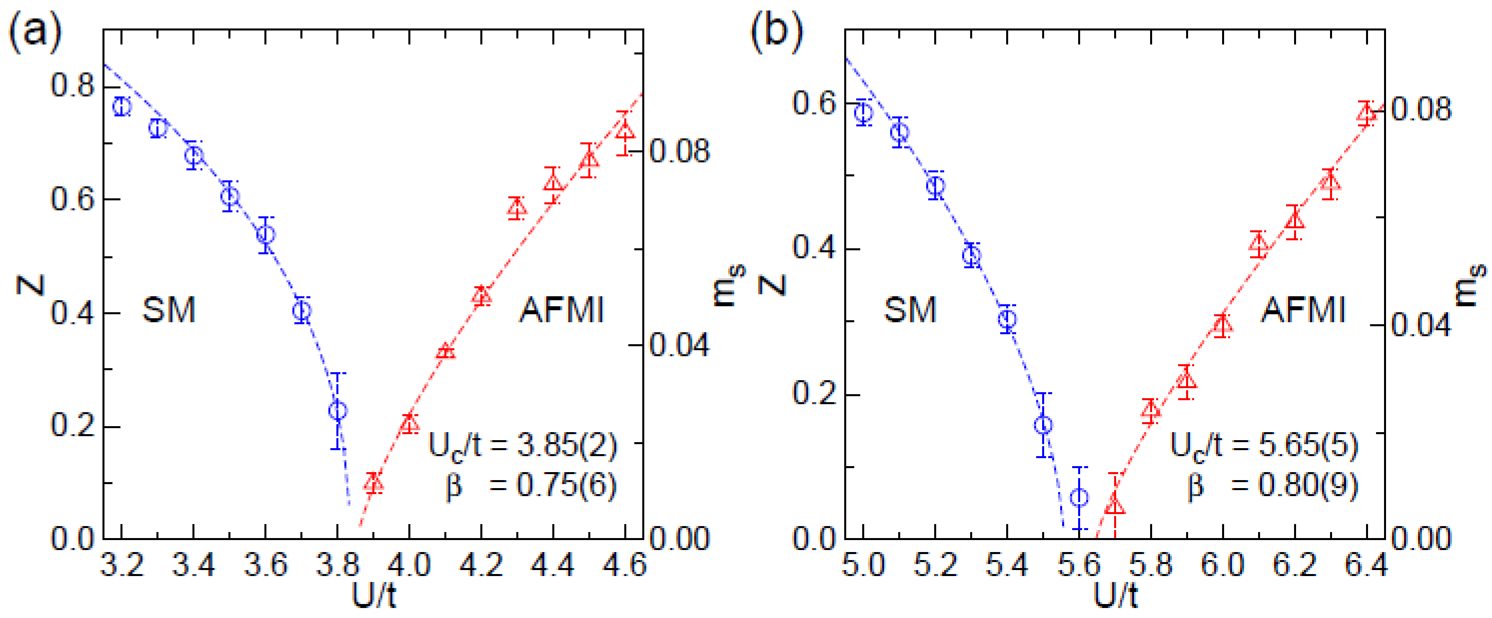
FIG. 6. Data collapse for the single particle gap. The exponents are taken for the ϵ-expansion of Ref. 6. (a) The crossing point pins down the value of U_c. (b) The data collapse again using $U_c/t = 3.78$. For comparison we have included the data for the magnetization.



Scaling of the quasiparticle weight:

(Otsuka, Yunoki, Sorella, PRX 2016)





Emerging picture of the Hubbard model:

1) Quality of scaling strongly suggests a direct, continuous transition, without an intermediate spin liquid phase. (corrections to scaling, Parisen Toldin, PRB 2015; larger sizes, Otsuki, PRX 2016)

2) Critical point seems to be in the Gross-Neveu universality class; boson's anomalous dimension is very large; (positive) fermion's anomalous dimension.

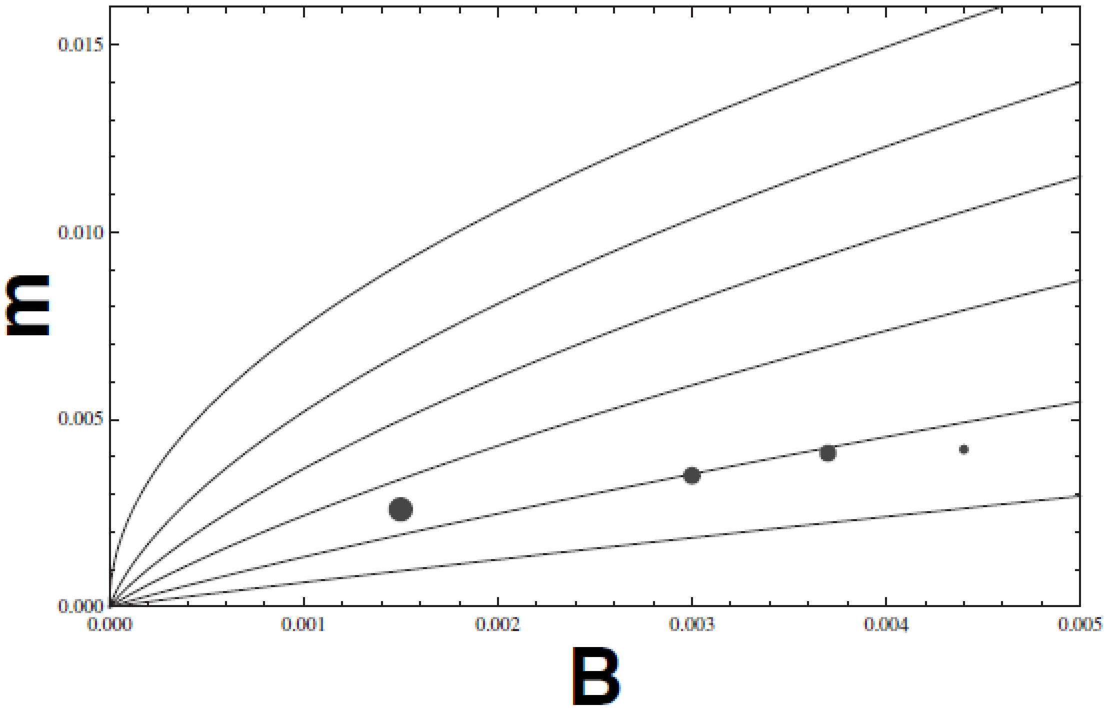
3) Reasonably good agreement with epsilon-expansion, some deviations do exist.

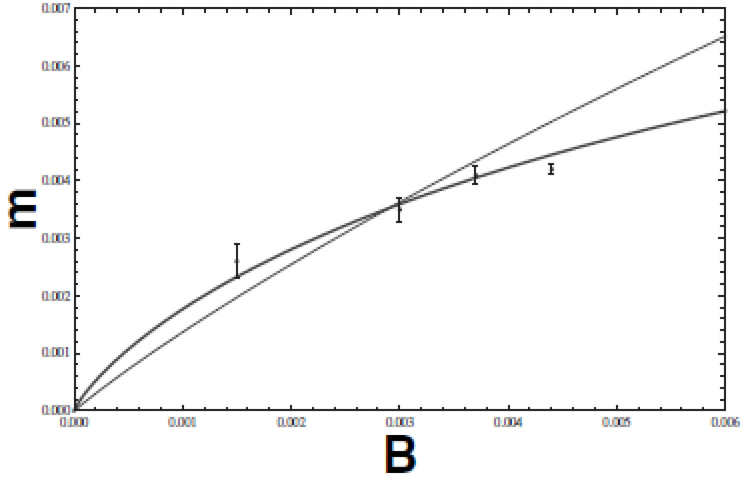
4) Lorentz invariance emergent , 1/r long-range tail marginally irrelevant. (numerically as well: Hohenadler, PRB 2014)

Scaling of the gap in the magnetic field: (IH, Roy, PRB 2008)

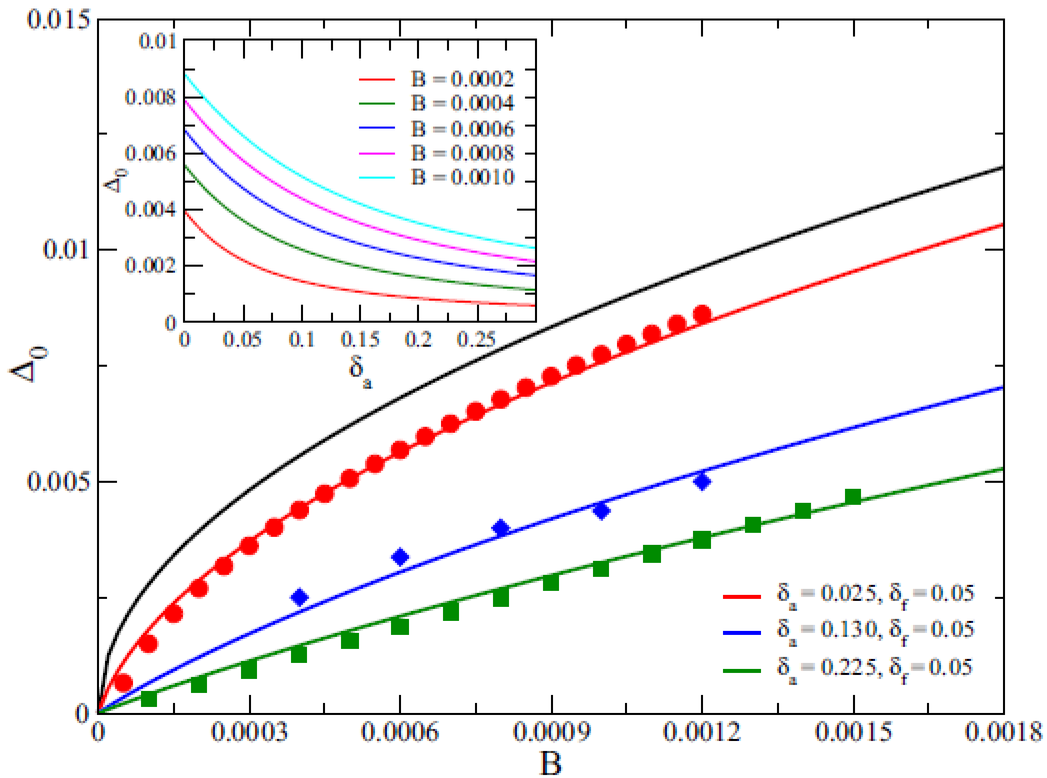
$$m = \frac{v_F}{l^z} G_+\left(\frac{l\delta^\nu}{a}, 0\right)$$

where **l** is the magnetic length, and G (0,0)= 1/5.985 + O(1/N).





More recently: (Roy, Kennett, Das Sarma, PRB 2014)

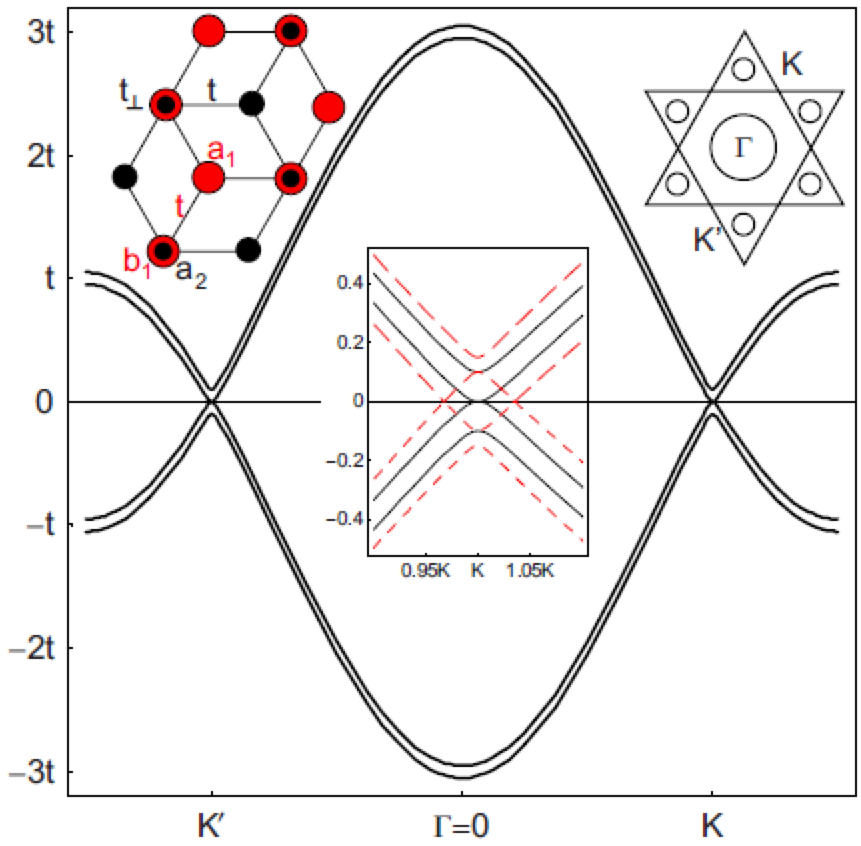


Graphene in the magnetic field is a canted AF! (Herbut, PRB 2007; Kharitonov, PRB 2012; Young, Nat. Phys. 2014)

2) Beyond graphene: quadratic band crossing

Bilayer graphene:

DOS is finite at the Fermi level in 2D => interactions decide the ground state



Single quadratic crossing point is now allowed: irreducible Hamiltonian (with time reversal):

$$\mathcal{H}_0(\mathbf{k}) = d_I I + d_x \sigma^x + d_z \sigma^z$$

with $d_I = t_I(k_x^2 + k_y^2), \; d_x = 2t_x k_x k_y, \; d_z = t_z(k_x^2 - k_y^2)$

With short-range interaction:

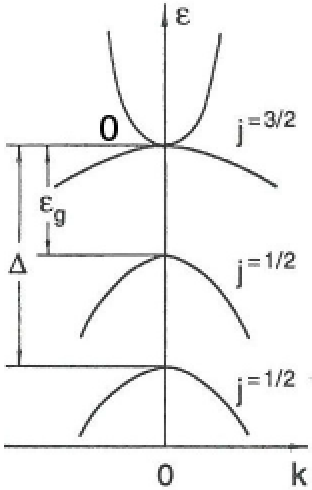
$$H = \int d\mathbf{r} \left[\mathbf{\Psi}^+(\mathbf{r}) H \mathbf{\Psi}(\mathbf{r}) + U \delta n_1(\mathbf{r}) \delta n_2(\mathbf{r}) \right]$$

has an instability at weak coupling:

$$\frac{dU}{d \ln s} = U^2 \rho_0 + O(U^3)$$

towards QAH (gapped) or nematic (gapless) phase. (Sun, PRL 2009, Vafek, PRB 2010, Lemonik, PRB 2010, Dora, PRB 2014)

Three dimensions: gapless semiconductors with band inversion (gray tin, HgTe, iridates(?))



Luttinger spin-orbit Hamiltonian (p-orbitals, J= 3/2) (Luttinger,1956)

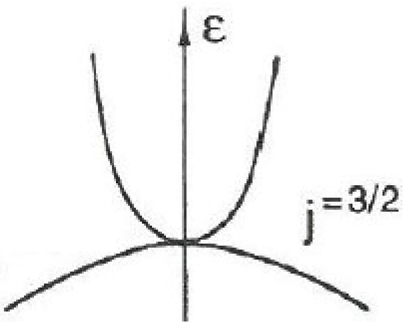
$$H = \frac{1}{2m}\left((\gamma_1 + \frac{5}{2}\gamma_2)k^2 - 2\gamma_2(\mathbf{k}\cdot\mathbf{S})^2\right)$$

with (rotationally symmetric) eigenvalues

$$E_L(k) = \frac{\gamma_1 + 2\gamma_2}{2m}k^2 \quad , \quad E_H(k) = \frac{\gamma_1 - 2\gamma_2}{2m}k^2$$

Luttinger Hamiltonian *à la* Dirac:

$$H(k) = \epsilon(\mathbf{k}) + \frac{\gamma_2}{m} d_a \Gamma^a$$



where,

$$\epsilon(\mathbf{k}) = \frac{\gamma_1}{2m} k^2, \;\; d_a(\mathbf{k}) = -3\xi_a^{ij} k_i k_j,$$
$$d_1 = -\sqrt{3}k_y k_z, \;\; d_2 = -\sqrt{3}k_x k_z, \;\; d_3 = -\sqrt{3}k_x k_y$$
$$d_4 = -\frac{\sqrt{3}}{2}(k_x^2 - k_y^2),$$
$$d_5 = -\frac{1}{2}(2k_z^2 - k_x^2 - k_y^2).$$

and five 4 x 4 Dirac matrices satisfy Clifford algebra:

$$\{\Gamma^a, \Gamma^b\} = 2\delta_{ab}$$

No sixth anticommuting matrix available: no mass term!

Without the hole band, at ``zero" (low) density:

Wigner crystal

With the hole band filled and particle band empty: the system is

critical

In the RG language, changing the cutoff causes the charge to ``flow"

$$\frac{de^2}{d\ln b} = (z+2-d)e^2 - 4e^4$$

(Abrikosov, ZETF (JETP) 1974; Moon, PRL 2013)

Below and near the upper critical dimension, $d_{up} = 4$, the system is in the non-Fermi liquid interacting phase, with the charge at the fixed point value:

$$e_*^2 = 15\epsilon/76 + \mathcal{O}(\epsilon^2)$$

with the small parameter

$$\epsilon = 4 - d$$

and the dynamical critical exponent $z < 2$.

$$z = 2 - \frac{16}{15}e^2$$

This implies power-laws in various responses, such as specific heat:

$$c_v \sim T^{d/z} \approx T^{1.7}$$

Easy way to get a NFL phase in 3D!

Or not?

The picture must somehow break down before the dimension reaches d = 2; a short range coupling flows like

$$\frac{dg_1}{d\ln b} = (z-d)g_1 \text{ + high. ord. term.}$$

and becomes marginal in d=2.

But, what can possibly happen to the NFL stable fixed point?

“Collision and annihilation”

The full interacting theory, with long-range and short-range interactions: (IH and Lukas Janssen, PRL 2014)

$$L = \Psi^\dagger \left(\partial_\tau + ia + d_i(-i\nabla)\gamma_i\right)\Psi + g_1(\Psi^\dagger\Psi)^2 + g_2(\Psi^\dagger\gamma_i\Psi)^2 + \frac{1}{2e^2}(\nabla a)^2$$

with Fierz constraint: $(\Psi^\dagger\gamma_i\gamma_j\Psi)^2 = 15(\Psi^\dagger\Psi)^2 + 2(\Psi^\dagger\gamma_i\Psi)^2$

Change of the cutoff now amounts to flow (one loop):

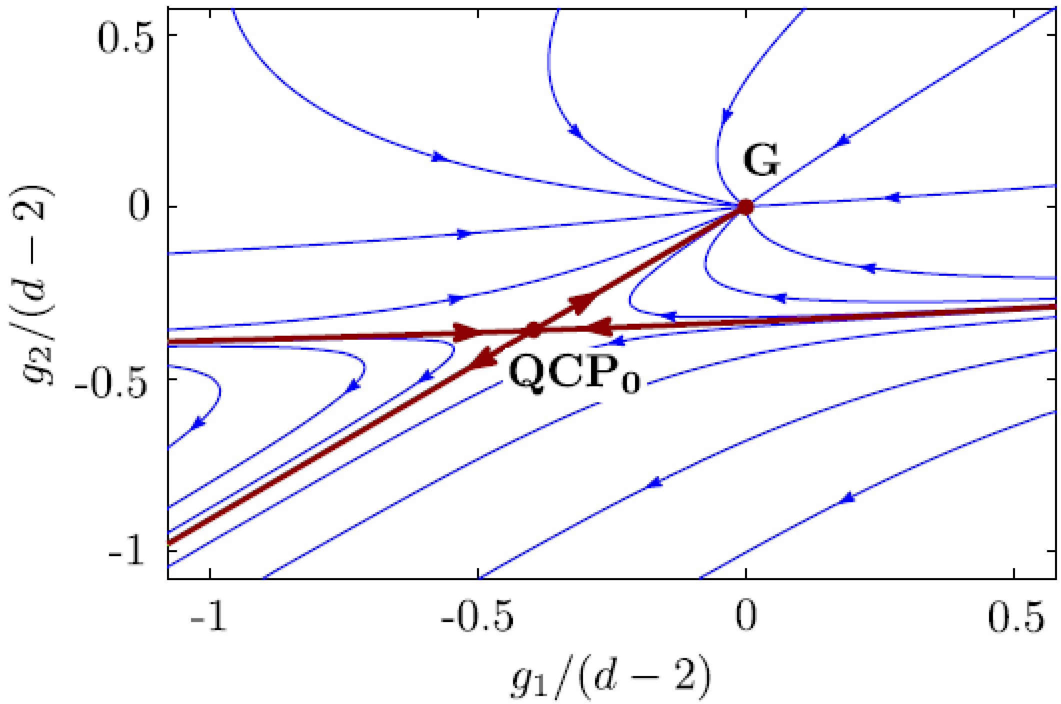
$$\frac{dg_1}{d\ln b} = (z-d)g_1 - \frac{1}{2}g_1 g_2 - \frac{5}{2}g_2^2 - 4e^2 g_2$$

$$\frac{dg_2}{d\ln b} = (z-d)g_2 + \frac{2}{5}g_1 g_2 - \frac{1}{20}g_1^2 - \frac{63}{20}g_2^2 - \frac{4}{5}e^2 g_1 + \frac{16}{5}e^2 g_2 - \frac{16}{5}e^4$$

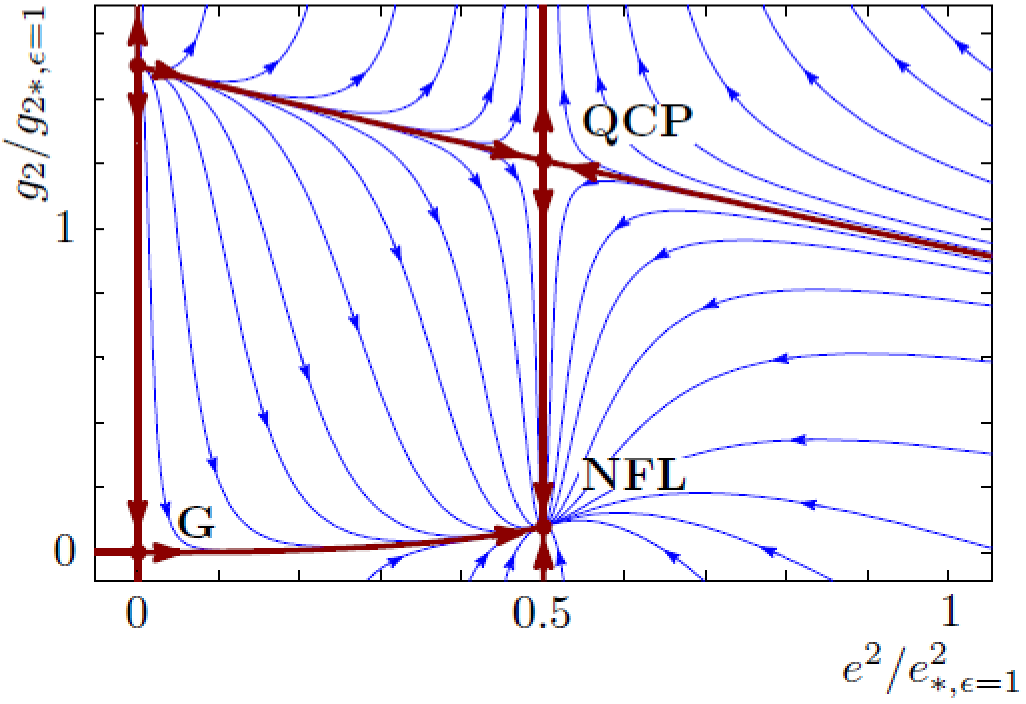
$$\frac{de^2}{d\ln b} = (z+2-d)e^2 - 4e^4$$

(Charge is here defined as: $e^2 = 2me_{\mathrm{el}}^2/(4\pi\hbar^2\varepsilon)$)

Without the long-range interaction (e=0), the theory possesses a quantum critical point (QCP_0); weakly coupled close to d=2:

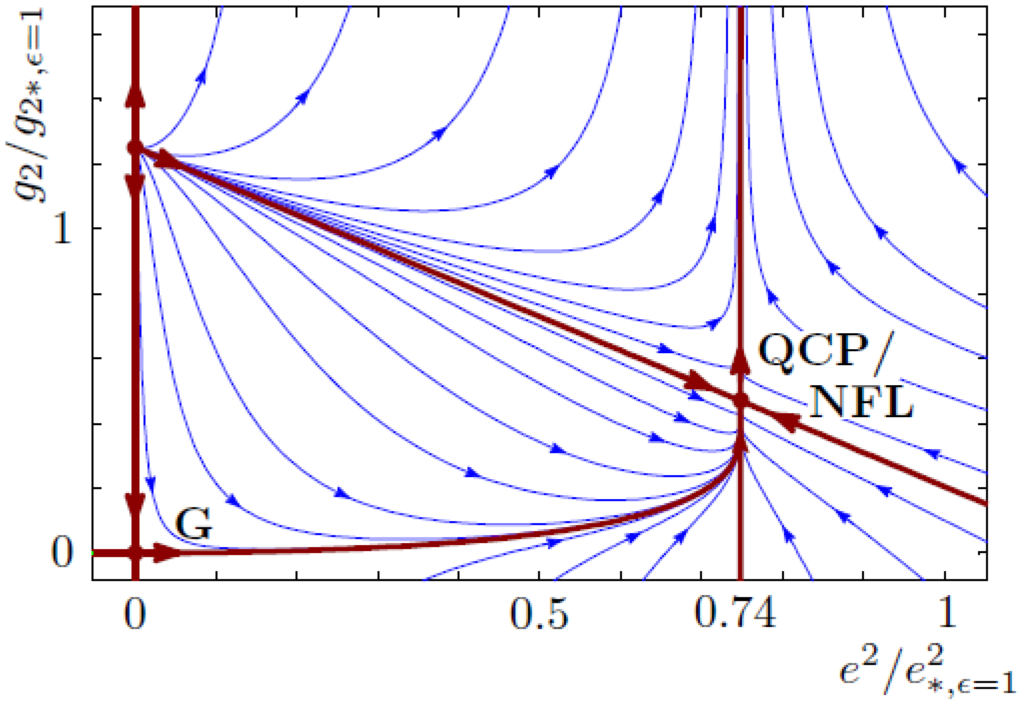


Close to and below d=4 there is a (IR stable) NFL fixed point, but also a (UV stable) quantum critical point at strong interaction:



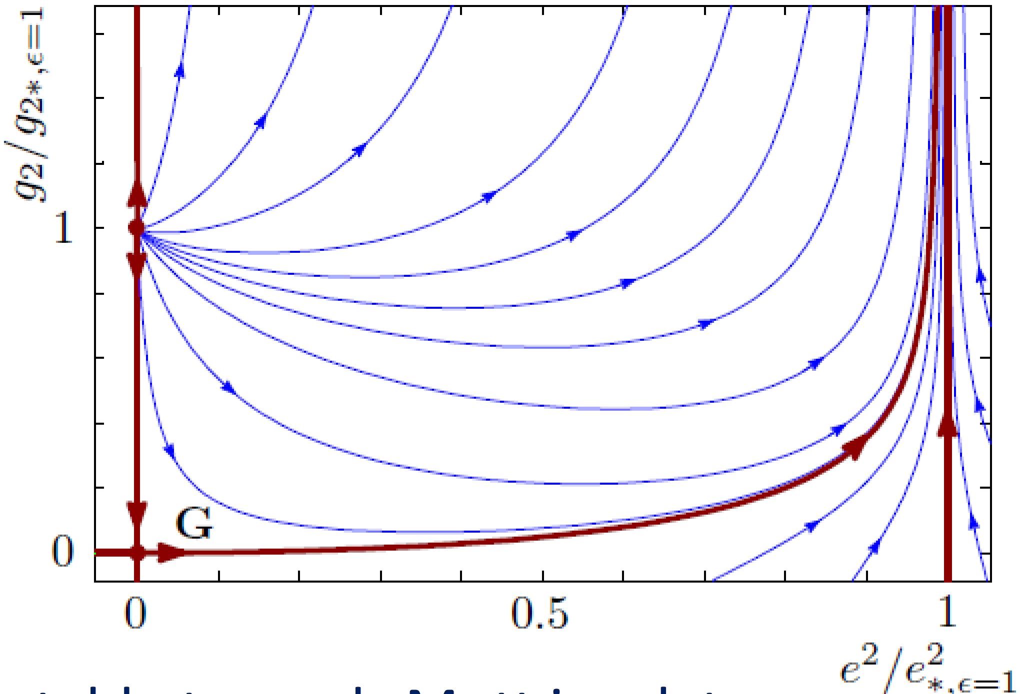
They get closer, but remain separated in the coupling space!

At some “lower critical dimension” NFL and QCP collide:



In one loop calculation, this occurs at $d_l = 3.26240$, slightly above three dimensions.

Finally, below dı the NFL and QCP become complex, and there is only a runaway flow left:



The system is unstable towards Mott insulator.

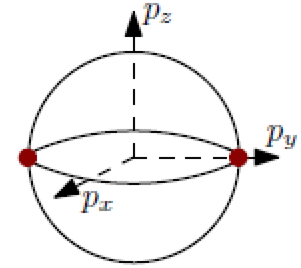
Scale invariance lost!

(Kaveh and IH, PRB 2005; Gies and Jaeckel 2006; Kaplan , PRD 2009)

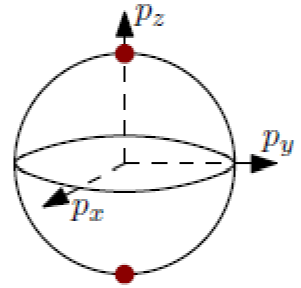
Order parameter for $d < d_{\rm low}$ $\qquad \chi_i = 2g_2\langle\Psi^\dagger\gamma_i\Psi\rangle$

Out of the five $\chi_1, \ldots, \chi_5$ not all equivalent:

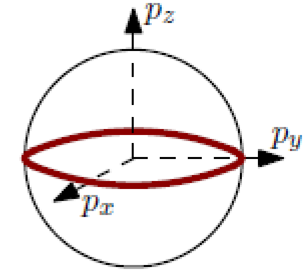
(1) $\chi_1 \neq 0$: $\varepsilon(\vec{p})$ gapped with minimal gap at two opposite points on equator



(2) $\chi_5 < 0$: $\varepsilon(\vec{p})$ gapless with gap closing at north and south pole



(3) $\chi_5 > 0$: $\varepsilon(\vec{p})$ gapped with minimal gap at entire equator



Energy $E = \int \frac{d\vec{p}}{(2\pi)^3}\varepsilon(\vec{p})$ is minimized for (3): $\chi_5 > 0$ (modulo O(3))

At large negative g_2 the system should develop anisotropic gap and,

$$\chi_5 > 0$$

The gap is minimal at the equator (in momentum space) at

$$p^2 = \chi_5/2$$

and the system looks as if under strain. The resulting ground state:

(topological) Mott insulator

(IH and Janssen, PRL 2014)

The state is equivalent in symmetry to ``uniaxial nematic”.

The fate of NFL: if d_l is above but close to d=3, the flow becomes slow close to (complex!) NFL fixed point. The RG escape time is long:

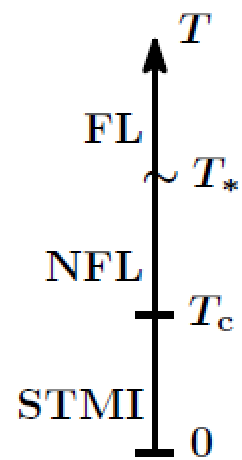
$$b_0 = e^{\frac{C}{\sqrt{d_{\rm low}-d}} - B + \mathcal{O}(d_{\rm low}-d)}$$

with non-universal constants C and B. There is wide crossover region of the NFL behavior within the temperature window

$$(T_{\rm c}, T_*)$$

with the critical temperature,

$$T_{\rm c} \approx T_* b_0^{-z}$$



Characteristic energy scale for interaction effects

$$k_{\rm B} T_* \sim \frac{e_{\rm el}^2}{\varepsilon L_*} = \frac{\hbar^2}{2m L_*^2} = \frac{4m}{m_{\rm el}\varepsilon^2} E_0$$

Assuming a small band mass

$$m/m_{\mathrm{el}} \approx 1/50$$

and a high dielectric constant

$$\varepsilon \approx 30$$

still gives a reasonable

$$T_* \sim 10\,\mathrm{K} - 100\,\mathrm{K}$$

and a detectable

$$T_{\mathrm{c}} \approx T_*/100$$

Further developments:

1) Yukawa-like field theory for the nematic (IR) critical point:
(Janssen & IH, PRB 2015)

$$L = L_\psi + L_{\psi\phi} + L_\phi$$

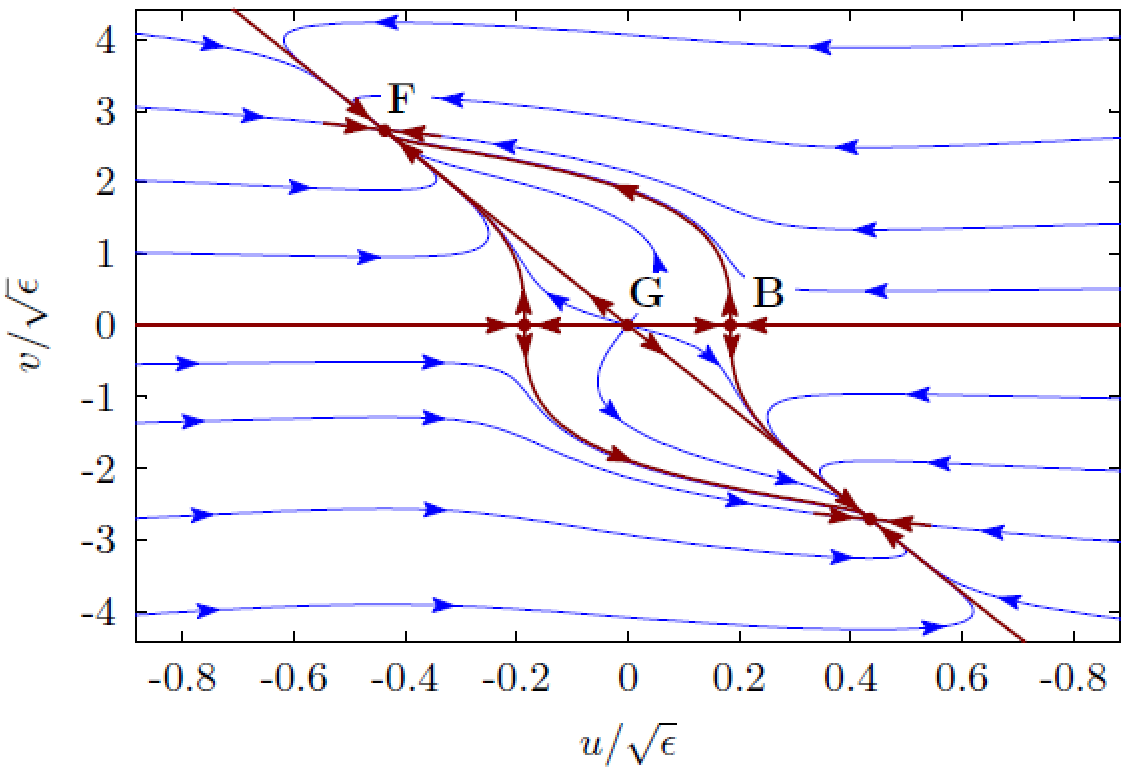
$$\begin{aligned} L_\psi &= \psi^\dagger \left(\partial_\tau + \gamma_a d_a(-i\nabla)\right)\psi, \\ L_{\psi\phi} &= g\phi_a \psi^\dagger \gamma_a \psi, \\ L_\phi &= \frac{1}{4} T_{ij}\left(-c\partial_\tau^2 - \nabla^2 + r\right) T_{ji} + \lambda T_{ij} T_{jk} T_{ki} \\ &\quad + \mathcal{O}(T^4). \end{aligned}$$

where the nematic tensorial order parameter is

$$T_{ij} = \phi_a \Lambda_{a,ij} \qquad \langle \phi_a \rangle = \frac{-g}{r} \langle \psi^\dagger \gamma_a \psi \rangle$$

And Λ_a are the five three dimensional Gell-Mann matrices.

RG flow, close to four (spatial) dimensions:



“B”: “classical” nematic critical point (Priest and Lubensky, 1976)

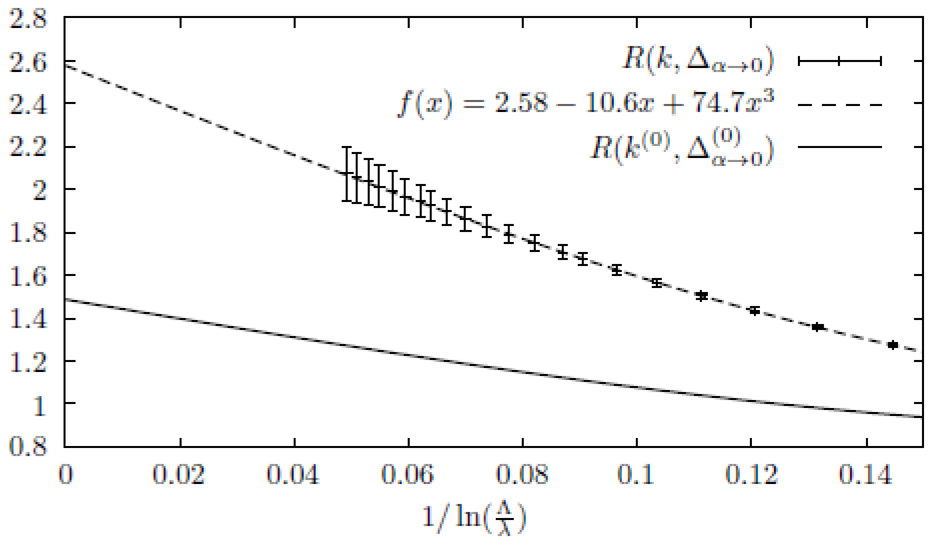
“F”: new fermionic fixed point

2) Large-N in three dimensions: (Janssen and IH, PRB 2016)

$N_c > 2.2$

Non-relativistic (integral) gap equation, variational approach:

Below N_c, rotational symmetry is broken!



Summary:

1) Emergent scale invariant non-fermi liquid phase in interacting Luttinger fermions, close to d=4

2) Mechanism of "fixed point collision and annihilation" could destabilize NFL phase in gapless semiconductors, and lead to breaking of O(3)

3) Analogous mechanism leads chiral symmetry breaking in QED_3,
(IH, arXiv:1605.09482)

4) Prediction: the characteristic separation of scales should be experimentally observable

5) Without the QCP scale-invariant phase is protected
(QED3 with a single Weyl fermion ?)

Thank you!