

New Frontiers For Interaction-Induced States

I P S I T A M A N D A L



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NORDITA

The Nordic Institute for
Theoretical Physics

Research Portfolio

Quantum Phase
Transitions
/ Unconventional
superconductivity
☛ 12 papers

Rényi Entropy
☛ 2 papers

Semimetals
/ Topological phases
☛ 16 papers

High Energy Physics
☛ 12 papers

Moiré superlattice
☛ 1 paper

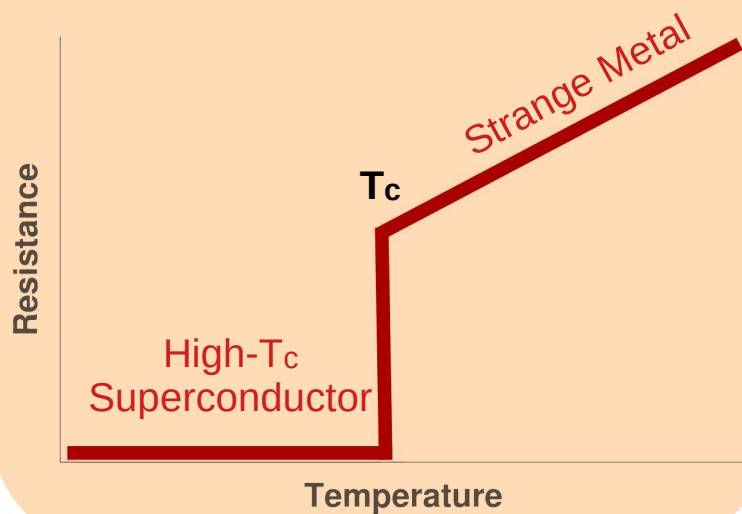
Miscellaneous:
Non-eqm dynamics,
quantum spin liquids,
transport properties, ...
☛ 7 papers

Quantum Condensed Matter
with focus on
Strongly Correlated Systems

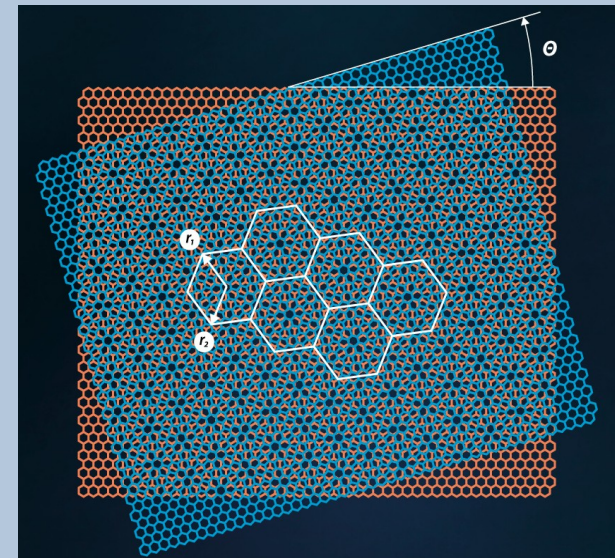
54 Papers
16 single auth.
16 major collabs.

Focal Points

Strange Metals or Non-Fermi liquids

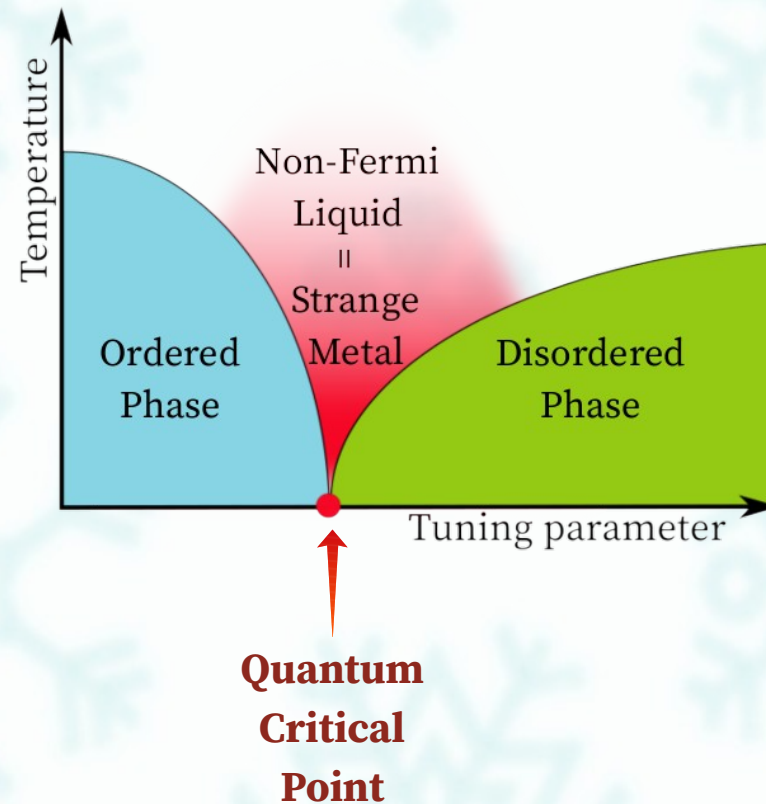


2d multi-layers ➡ Moiré superlattices



MIPT

Strange Metals from Quantum Critical Points



Theory of Normal Metals

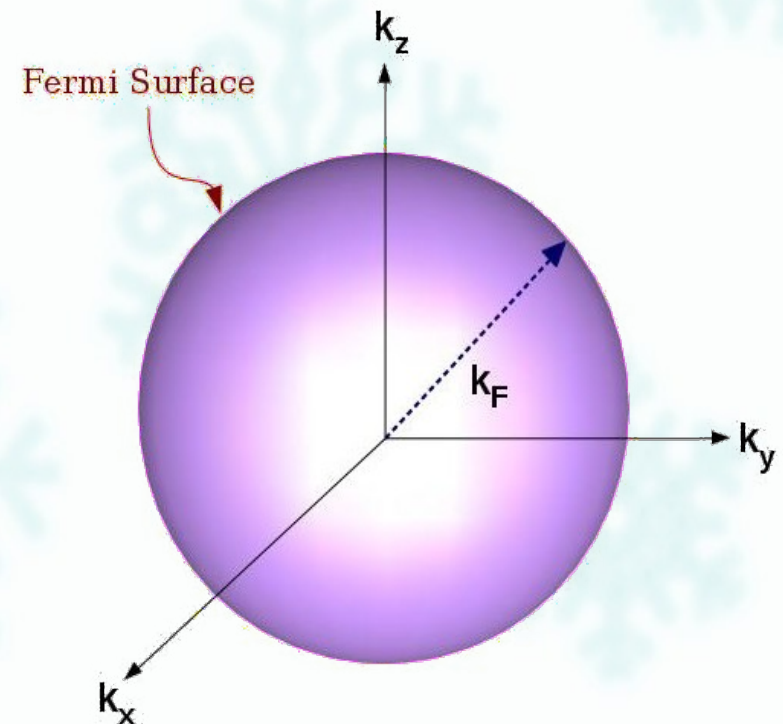
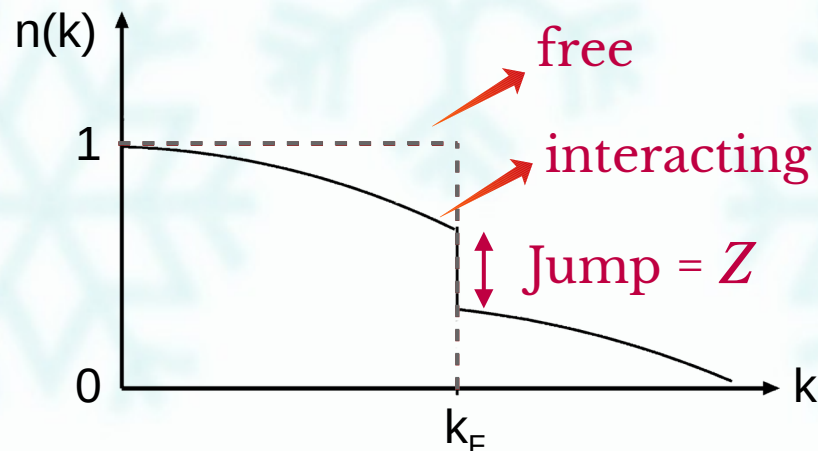


Landau

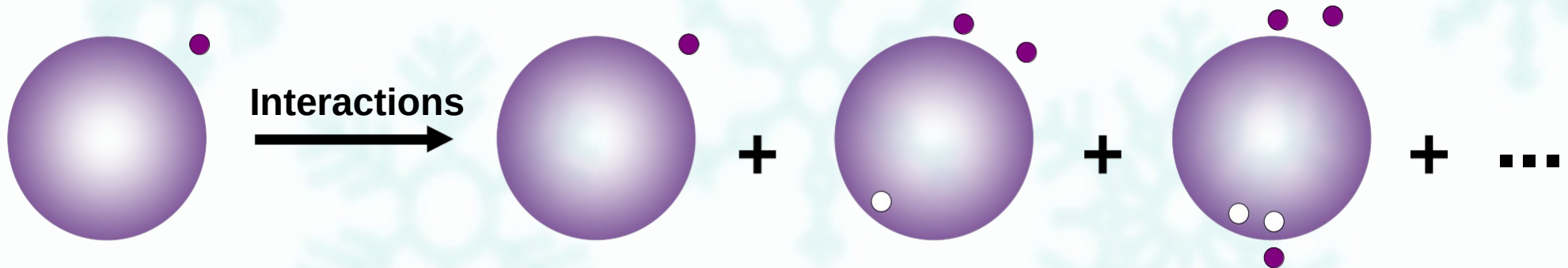
Fermi Liquid (FL) • Properties of finite density interacting fermions don't depend on specific microscopic details

- **Ground state** • characterized by a sharp Fermi surface (FS) in momentum space
- **Quasiparticles** • low energy excitations near FS

FS • jump in fermion occupation number $n(k)$ at $T=0$



Quasiparticles: Emergent Entities in FL



Coherent part of
single-particle Green's function

$$G_R(\omega, \mathbf{k}) = \frac{Z}{\omega - v_F k_{\perp} - k_{\parallel}^2 + i\Gamma}$$

$$\omega = E - E_F, \quad k_{\perp} = k - k_F$$

Quasiparticles

• collective low energy
quantum oscillations

- ✓ Quasiparticle lifetime diverges close to FS • Decay rate $\Gamma \sim \omega^2$
- ✓ Overlap between elementary excitations of free and interacting systems • quasiparticle weight $0 < Z \leq 1$

Manifestation of FL

- Ground state adiabatically connected to the non-interacting problem
- Quasiparticles $\xleftrightarrow{\text{one-to-one}}$ free system excitations
- Temperature (T) dependence of thermodynamic & transport properties similar to free fermions

- Resistivity $\rho \propto T^2$
- Specific heat $\propto T$
- Im (self energy Σ) $\propto \omega^2$

A complicated problem reduced to a simpler one

Breakdown of FL Theory

Long-lived
quasiparticles

FL

Massive

Electrons + Bosons

Massless

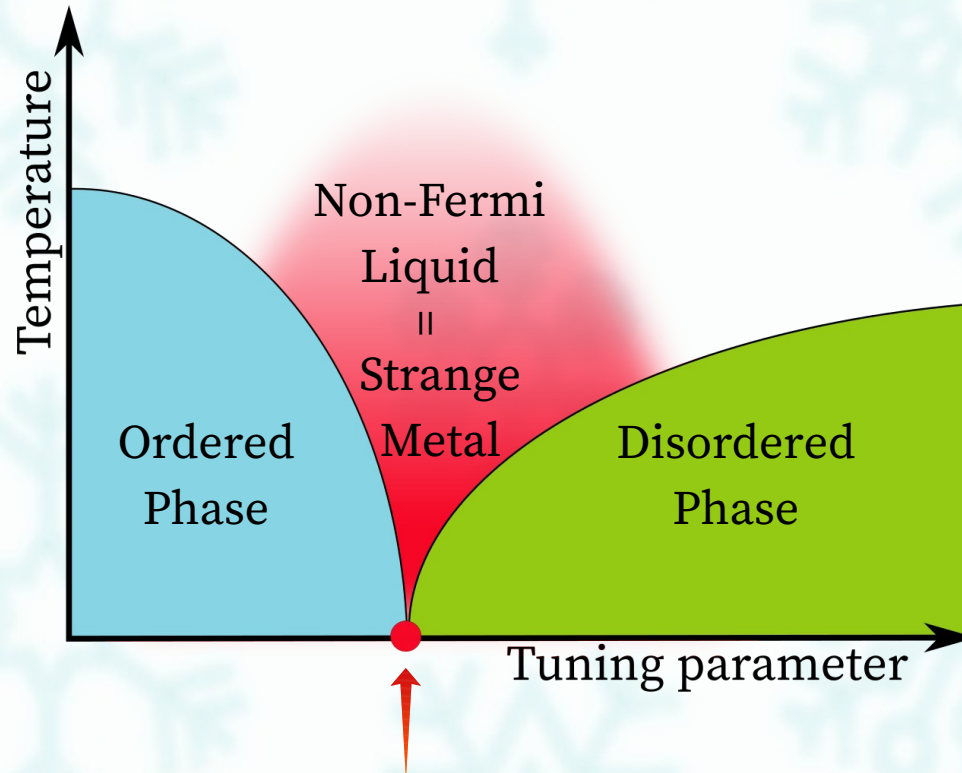
Low energy QFT

Boson

Boson

No quasiparticle

non-Fermi liquid
(NFL)



Bosonic order parameter
massless at
Quantum Critical Point
(QCP)

mediates

strong
interactions

e.g. Antiferro order,
nematic order,
charge density order,
gauge fields ...

Quantum Critical Metal

Recipe for NFL as fermion-boson coupling becomes strong in 2d, even if bare coupling is weak $\rightarrow Z \rightarrow 0$ quasiparticles destroyed

FL **FS away from QCP**



NFL

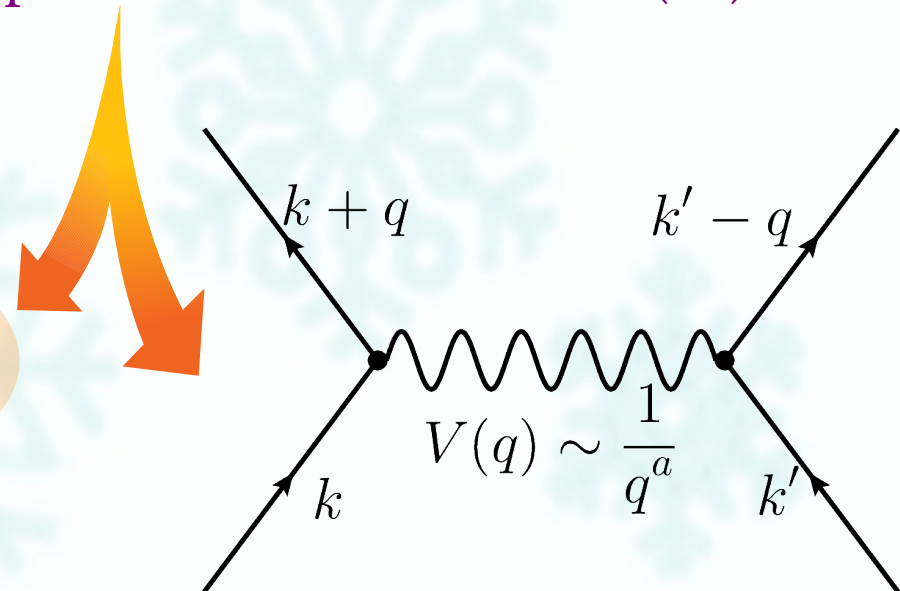
FS at QCP



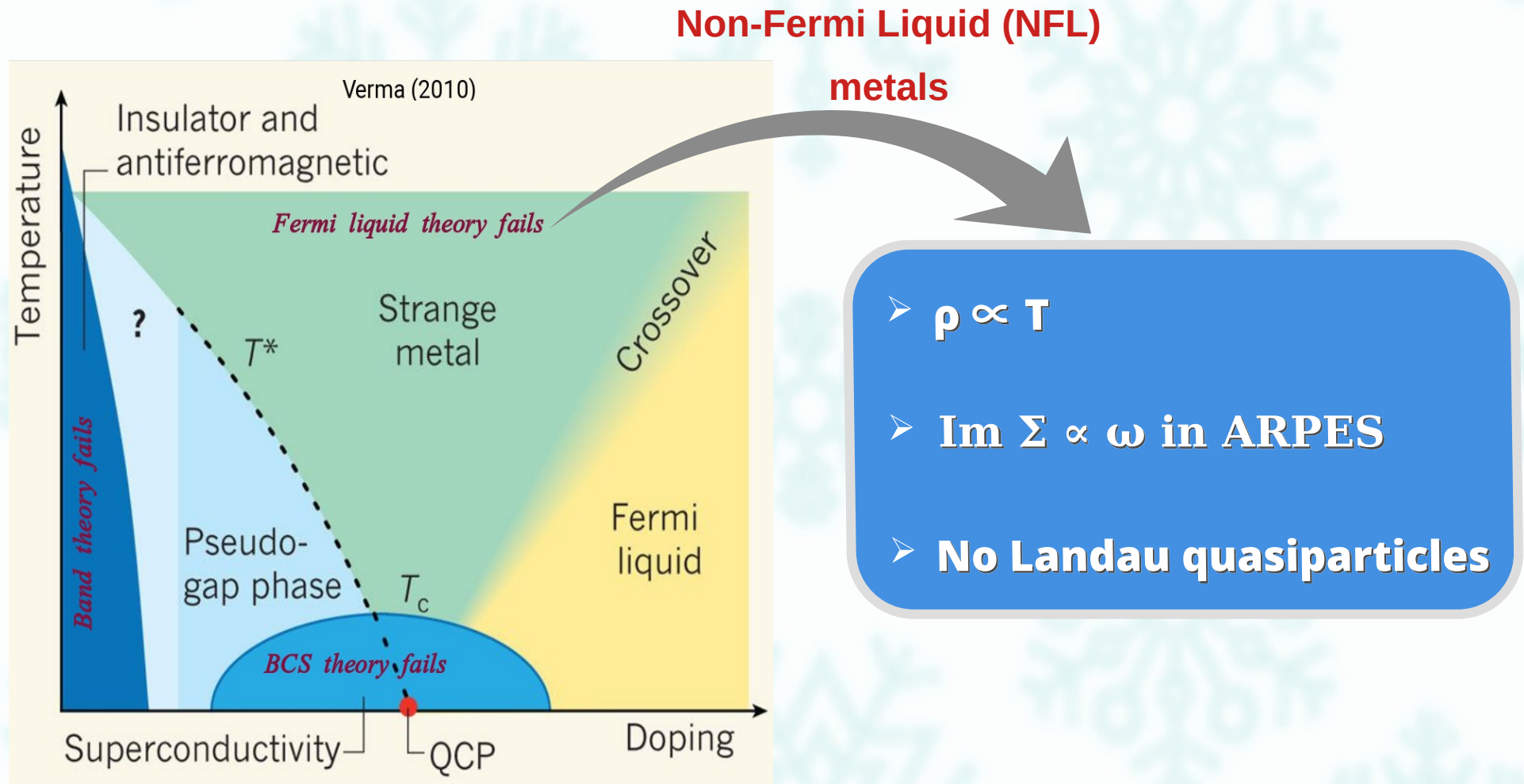
Critical fluctuations at QCP coupled to itinerant electrons (FS)

Attempt to describe NFL as

FS + Gapless Order Parameter fluctuations



Where do NFLs Appear?



Phase diagram of high- T_c cuprates

NFLs: How to Explain Theoretically?

We developed a novel analytical framework



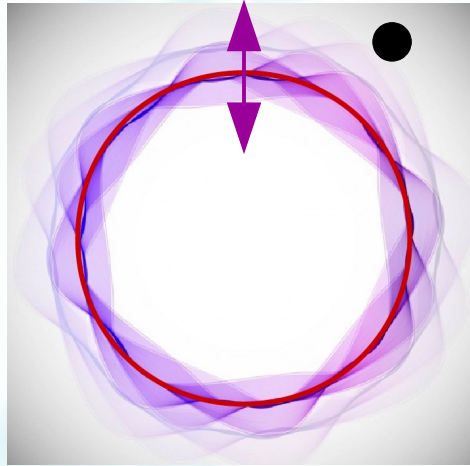
QFT

Dimensional Regularization + Renormalization Group

[**IM** & S-S Lee, *PRB* (2015)]

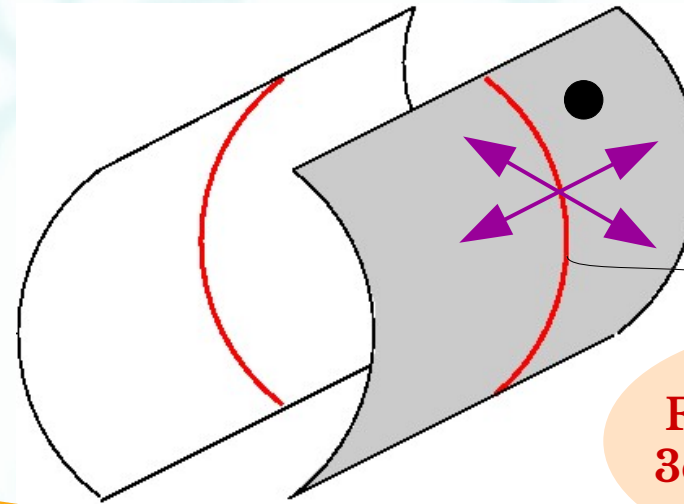
**Our controlled approximation allowed to compute
critical exponents, optical conductivity, ...**

NFLs: Dimensional Regularization



FS of
2d metal

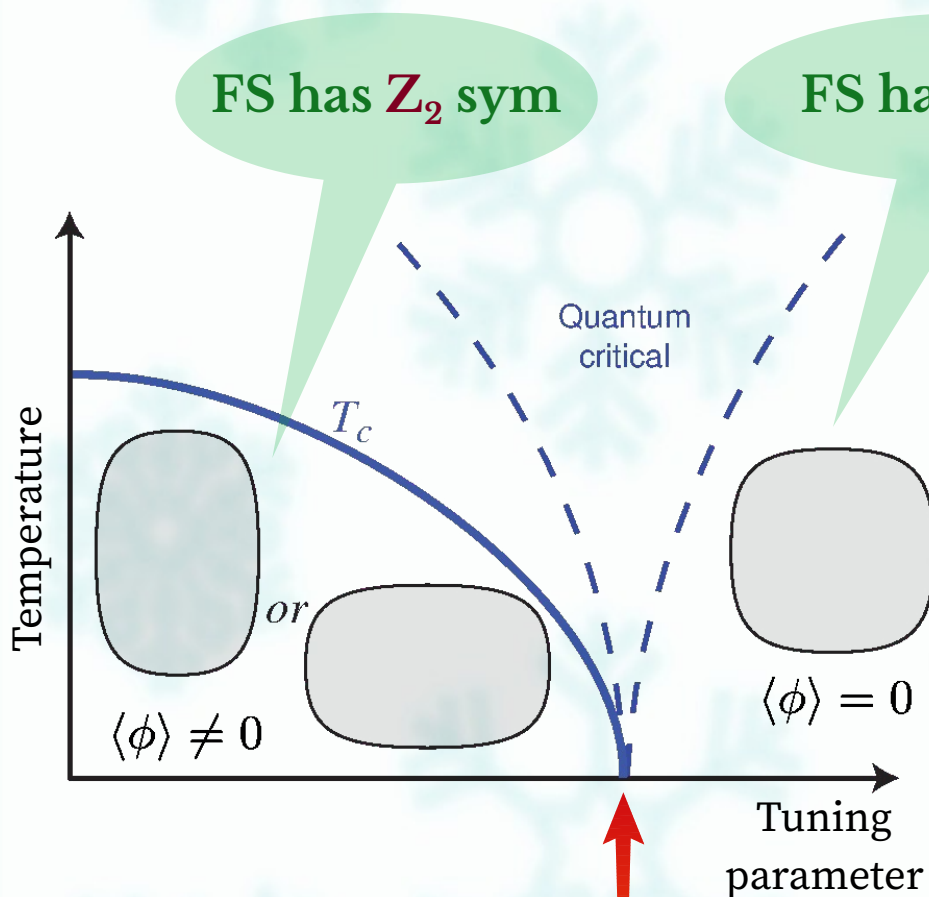
Suppress qtm
fluctuations
by adding extra
dimensions
 $\perp$ FS



Fermi line in
3d mom space

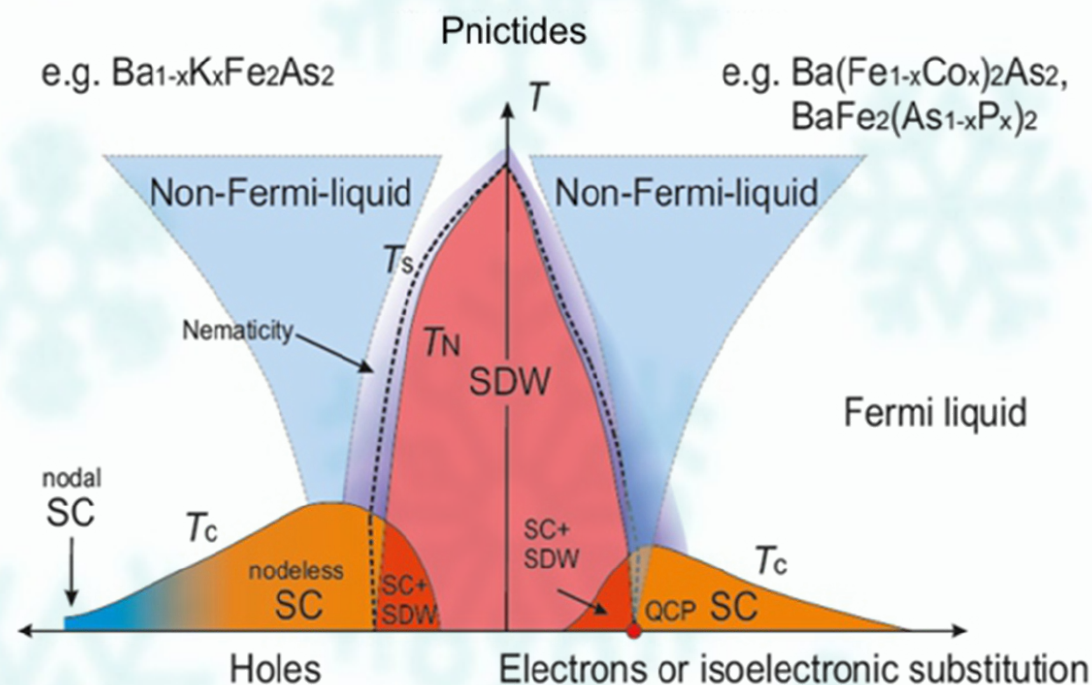
- Find upper critical dimension d_c such that $d > d_c$ described by mean-field theory (FL) • well-known tool from Statistical Mechanics / QFT
- $d_{\text{phys}} \leq d_c$ • mean-field theory inapplicable
• carry out perturbation in $\epsilon = d_c - d_{\text{phys}}$

Applications: Ising-Nematic QCP



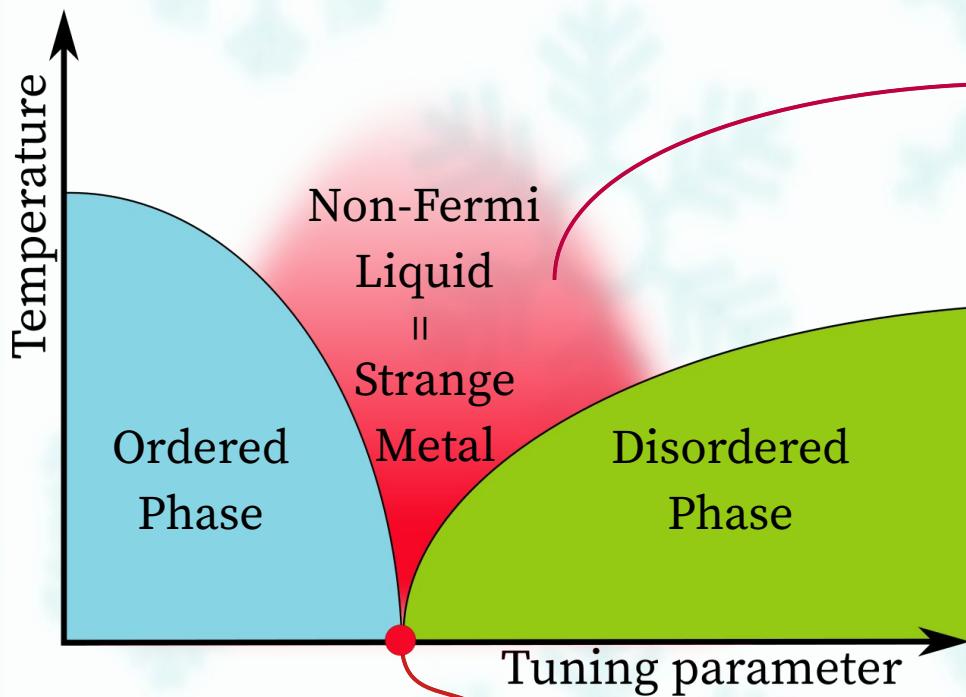
Massless
at QCP

Order Parameter ϕ $\rightarrow$ Real Scalar Boson



[**$\text{YBa}_2\text{Cu}_3\text{O}_y$** (Cuprate), **$\text{Sr}_3\text{Ru}_2\text{O}_7$** (Ruthenate), **Pnictides**]

Results: 2d Ising-Nematic QCP



**Massless Boson at
Quantum Critical Point**

1d FS fluctuations
effectively local

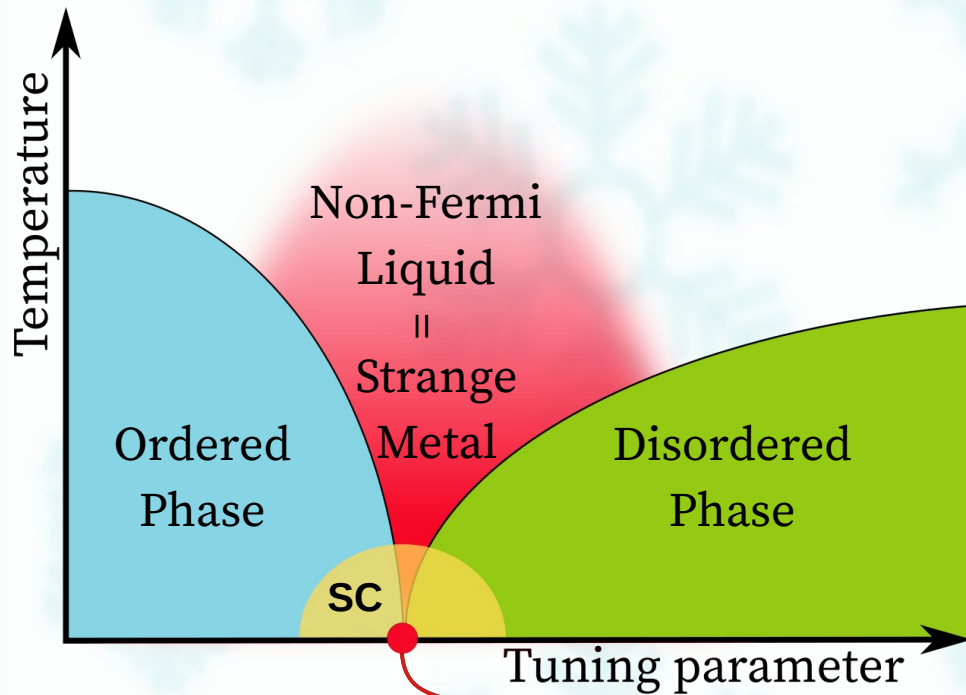
Optical conductivity

$$\sigma(\omega) \sim \omega^{-2/3}$$

☛ close to $\omega^{-0.65}$ found in expts.
on optimally doped cuprates

[A. Eberlein, **IM**, & S. Sachdev,
PRB (2016)]

Results: 2d Ising-Nematic QCP



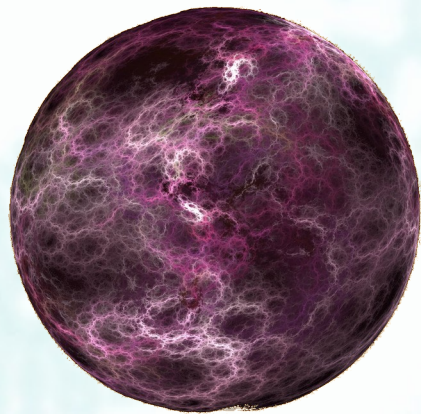
Quantum Critical Point
masked by superconducting
(SC) dome

**Competition between
non-Fermi liquid phase
&
pairing instability at $T=0$**

☛ **Superconductivity (SC) wins**

[**IM**, *PRB* (2016)]

Results: 3d Ising-Nematic QCP



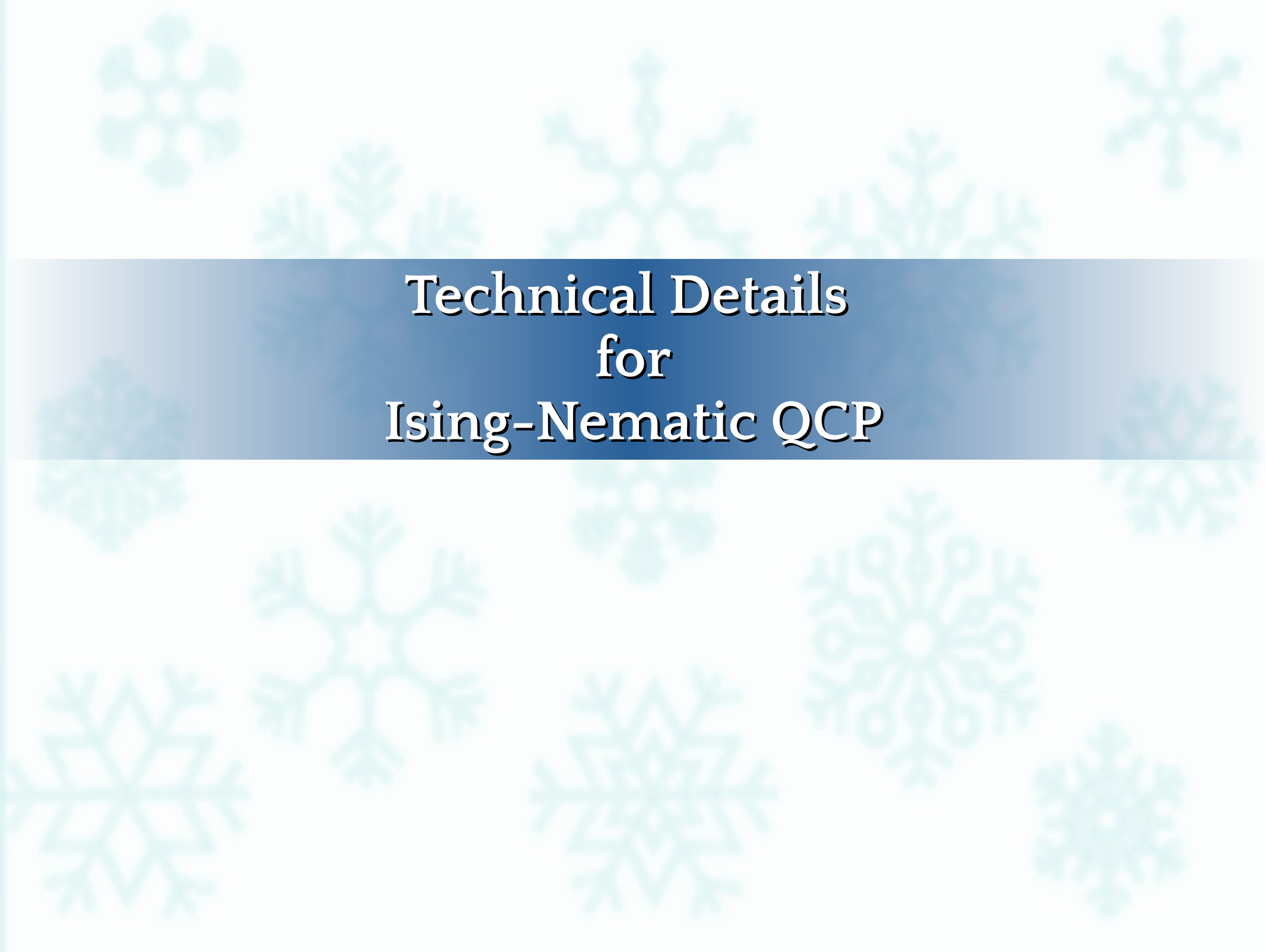
2d FS fluctuations
non-local

☞ entangled all over the FS

- **Fluctuations less violent than 1d FS**
- **Ultraviolet / Infrared mixing**
- **≥ 2 -loop corrections vanish**

[**IM** & S-S Lee, *PRB* (2015)]

[**IM**, *EPJB* (2016)]

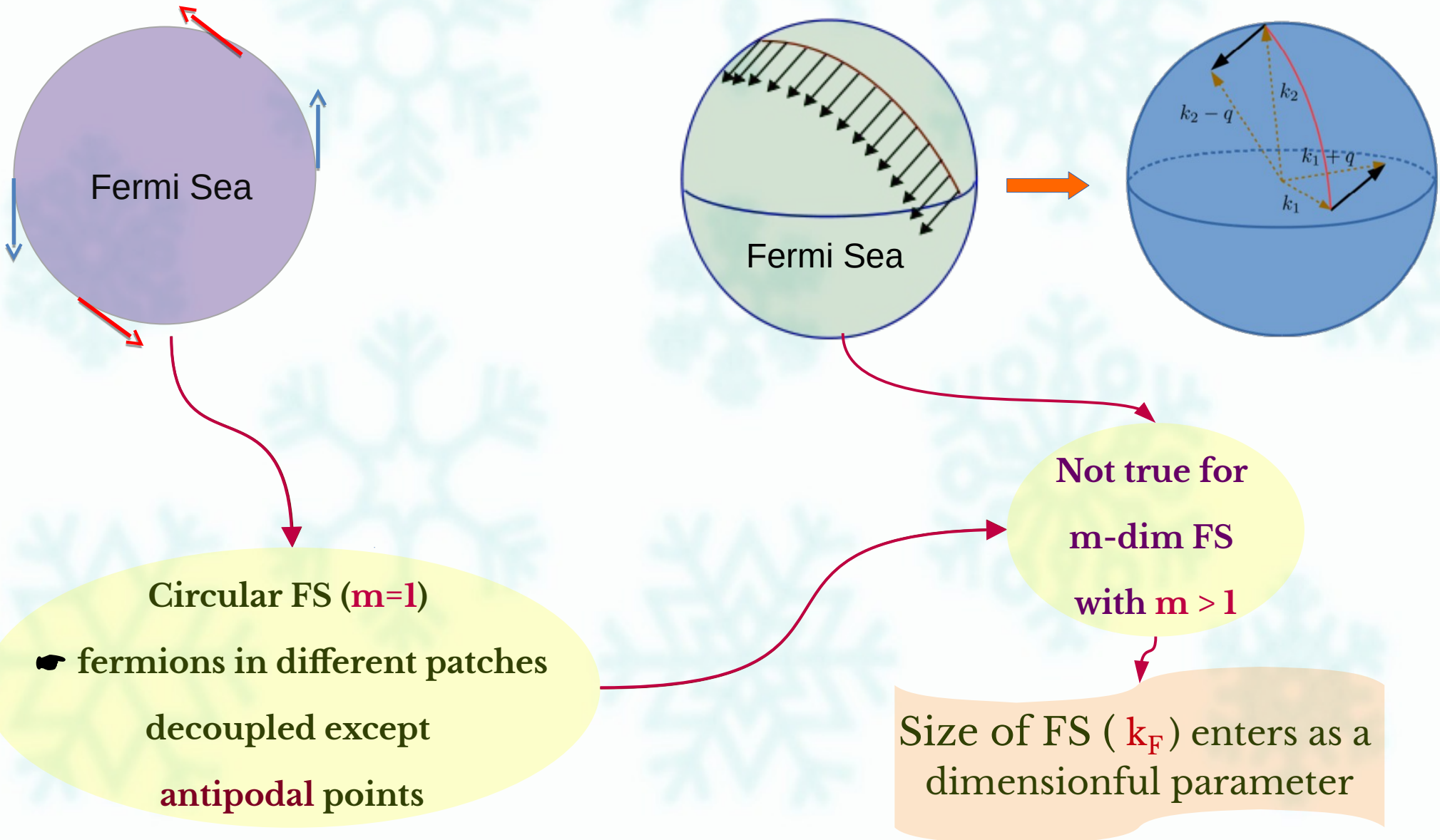


Technical Details for Ising-Nematic QCP

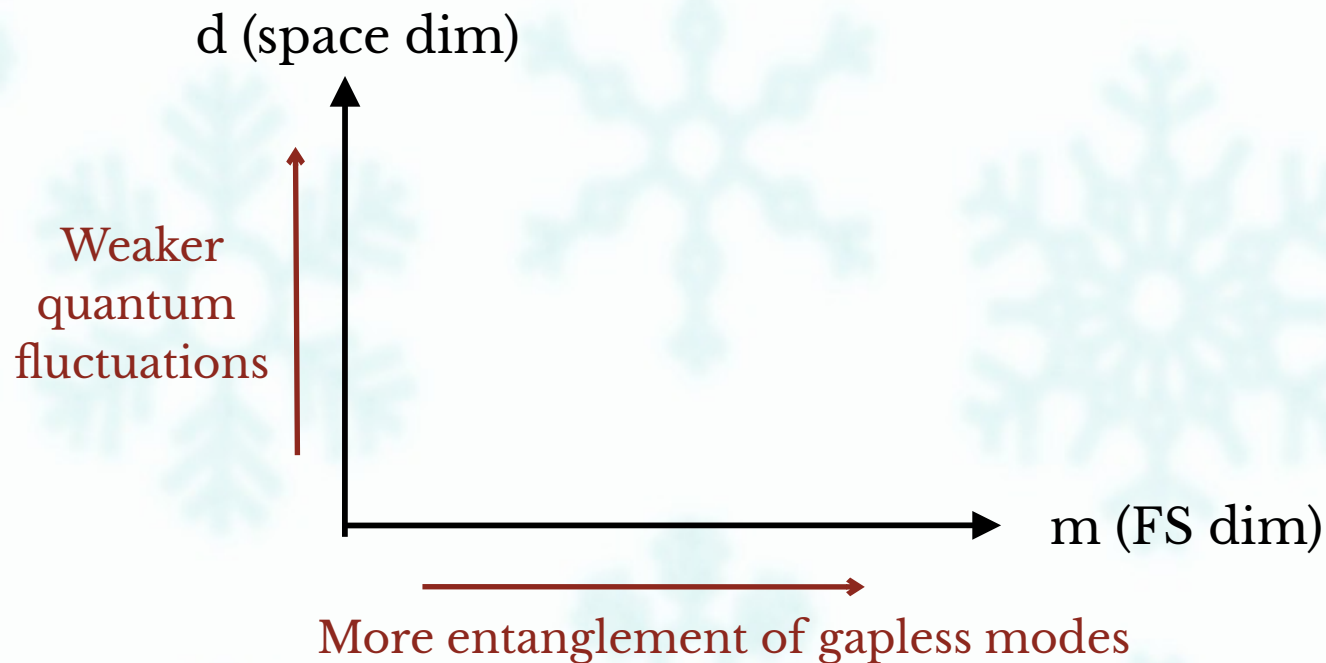
m-dim FS + Scalar Boson

Low energy limit $\rightarrow$ Fermions scatter tangentially

Time-Reversal Invariance assumed



Significance of m

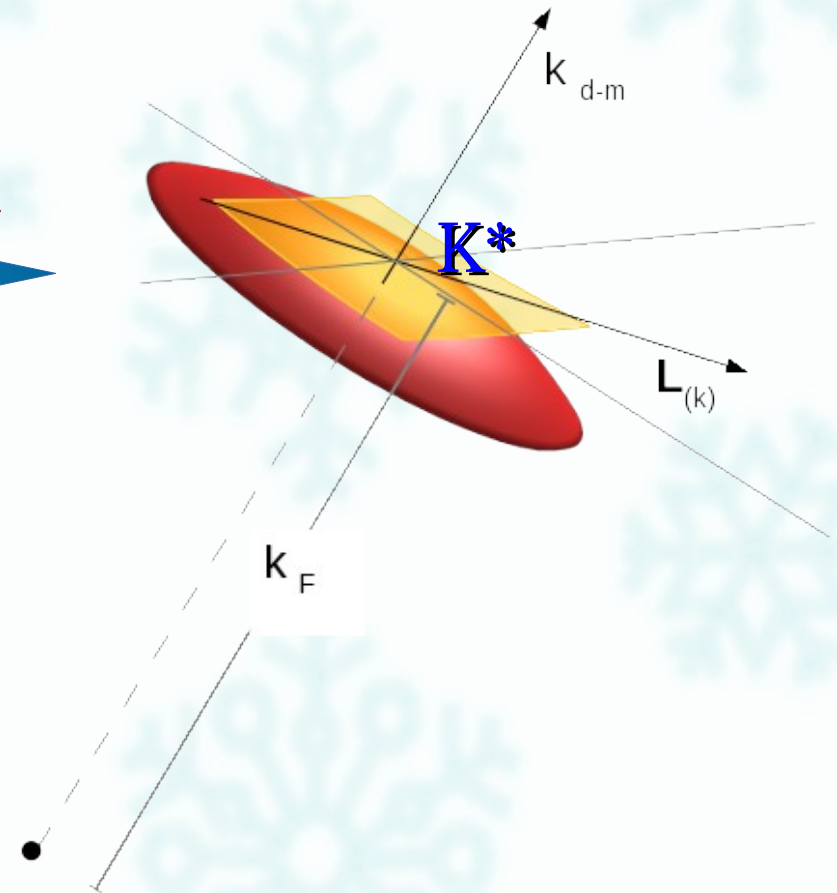


- $m = 1$ ➡ observables local in mom space (e.g. Green's fns) can be extracted from local patches ➡ emergent locality
[D. Dalidovich & S-S. Lee, *Phys. Rev. B* 88, 245106 (2013)]
- $m > 1$ ➡ UV/IR mixing ➡ low-energy physics affected by gapless modes on entire FS ➡ size of FS (k_F) modifies naive scaling coming from patch description ➡ k_F becomes a 'naked scale'
[**IM** & S-S Lee, *Phys. Rev. B* 92, 035141 (2015)]

Coordinate Set-up

Patch of m -dim FS
of arbitrary shape

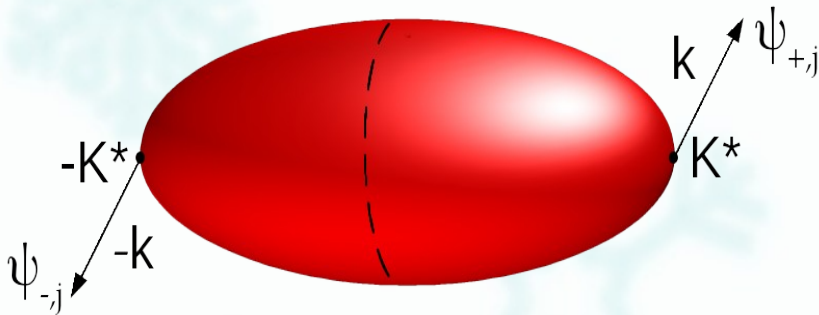
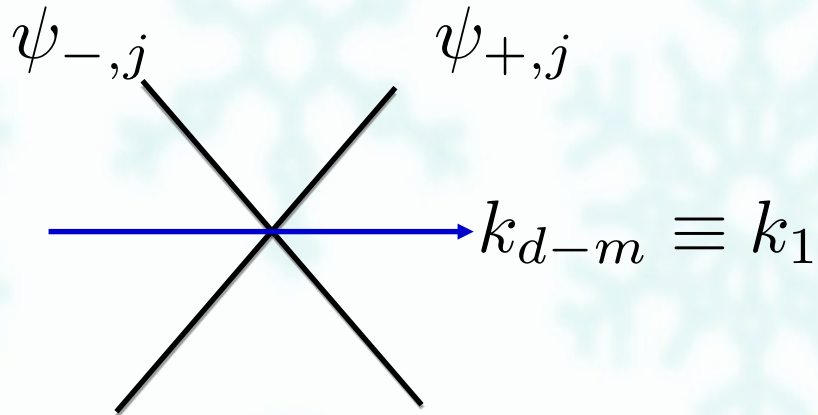
$$d = d_{\text{phys}} = m + 1$$



- At a chosen point K^* on FS : $k_{d-m} \perp \text{local } S^m$ $\Rightarrow$ its magnitude measures deviation from k_F
- $L_{(k)} = (k_{d-m+1}, k_{d-m+2}, \dots, k_d)$ $\Rightarrow$ tangential along the local S^m

Fermions on Antipodal Points

Time-Reversal Invariance assumed



$\psi_{+,j} (\psi_{-,j})$



right (left) moving fermion
with flavour $j=1,2,\dots,N$

Effective Action

2 halves of m-dim FS
+ massless boson
in d space
& one time dim

↓ $d = d_{\text{phys}} = m + 1$

$$\begin{aligned}
 S = & \sum_{s=\pm,j} \int \frac{d^{m+2}k}{(2\pi)^{m+2}} \psi_{s,j}^\dagger(k) \left[i k_0 + s k_{d-m} + \mathbf{L}_{(k)}^2 \right. \\
 & \left. - \mathcal{O}(|\mathbf{L}_{(k)}|^3) \right] \psi_{s,j}(k) \\
 & + \frac{1}{2} \int \frac{d^{m+2}k}{(2\pi)^{m+2}} \left[k_0^2 + k_1^2 + \mathbf{L}_{(k)}^2 \right] \phi(-k) \phi(k) \\
 & + \frac{e}{\sqrt{N}} \sum_{s=\pm,j} \int \frac{d^{m+2}k d^{m+2}q}{(2\pi)^{2m+4}} \phi(q) \psi_{s,j}^\dagger(k+q) \psi_{s,j}(k)
 \end{aligned}$$

Action in terms of Dirac Fermions

$$\Psi_j(k) = \begin{pmatrix} \psi_{+,j}(k) \\ \psi_{-,j}^\dagger(-k) \end{pmatrix}$$

Interpret $|\mathbf{L}_{(k)}|$ as a continuous flavour
 • each $(m+2)$ -d spinor can be viewed as a $(1+1)$ -d Dirac fermion



$$\begin{aligned} S = & \sum_j \int \frac{d^{m+2}k}{(2\pi)^{m+2}} \bar{\Psi}_j(k) i \left[\gamma_0 k_0 + \gamma_1 \left(k_{d-m} + \mathbf{L}_{(k)}^2 \right) \right] \Psi_j(k) \\ & + \frac{1}{2} \int \frac{d^{m+2}k}{(2\pi)^{m+2}} \mathbf{L}_{(k)}^2 \phi(-k) \phi(k) \\ & + \frac{i e}{\sqrt{N}} \sum_j \int \frac{d^{m+2}k d^{m+2}q}{(2\pi)^{2m+4}} \phi(q) \bar{\Psi}_j(k+q) \gamma_{d-m} \Psi_j(k) \end{aligned}$$

Embed FS in Higher Dimensions

Add extra spatial dimensions $\perp \mathbf{L}_{(k)}$

• $d > d_{\text{phys}}$

$$k_0 \rightarrow \mathbf{K} \equiv (k_0, k_1, \dots, k_{d-m-1})$$

$$\gamma_0 \rightarrow \Gamma \equiv (\gamma_0, \gamma_1, \dots, \gamma_{d-m-1})$$

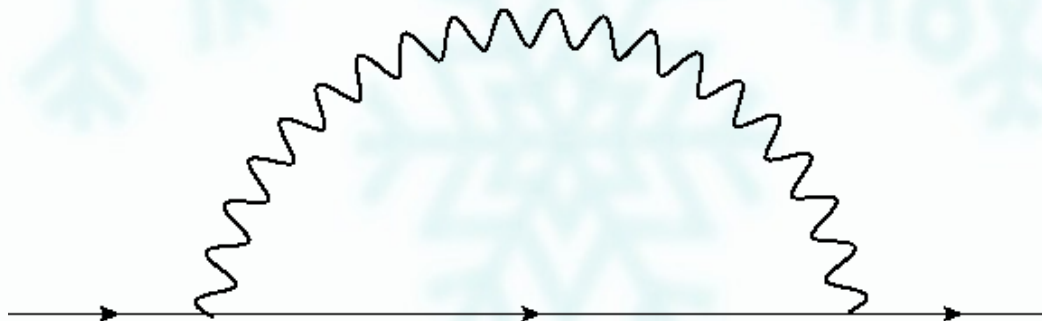
$$\gamma_1 \rightarrow \gamma_{d-m}$$

$$\delta_k \equiv k_{d-m} + \mathbf{L}_{(k)}^2$$

$$\begin{aligned}
 S = & \sum_j \int \frac{d^{d+1}k}{(2\pi)^{d+1}} \bar{\Psi}_j(k) \, i \left[\mathbf{\Gamma} \cdot \mathbf{K} + \gamma_{d-m} \delta_k \right] \Psi_j(k) \\
 & + \frac{1}{2} \int \frac{d^{d+1}k}{(2\pi)^{d+1}} \mathbf{L}_{(k)}^2 \phi(-k) \phi(k) \\
 & + \frac{i e}{\sqrt{N}} \sum_j \int \frac{d^{d+1}k \, d^{d+1}q}{(2\pi)^{2d+2}} \phi(q) \bar{\Psi}_j(k+q) \gamma_{d-m} \Psi_j(k)
 \end{aligned}$$

Energy Scales

- Λ is implicit UV cut-off with $\mathbf{K}, \mathbf{k}_{d-m} \ll \Lambda \ll \mathbf{k}_F$
- $\mathbf{k}_F$ $\rightarrow$ sets FS size
 Λ $\rightarrow$ sets the largest momentum fermions can have $\perp$ FS
- Renormalization Group (RG) flows $\rightarrow$ change Λ
 & require low-energy observables independent of Λ
- Fix $\mathbf{m}$ & tune $\mathbf{d}$ towards $\mathbf{d}_c$ at which fermion self-energy diverges logarithmically in Λ $\rightarrow$ access NFL perturbatively in $\epsilon = \mathbf{d}_c - (\mathbf{m}+1)$



Critical Dimension

- Upper critical dim $\Rightarrow d_c = m + \frac{3}{m+1}$

$$d_c = 3 \quad \text{for } (m = 2, d_{phys} = 3)$$

$$d_c = 5/2 \quad \text{for } (m = 1, d_{phys} = 2)$$

- Scaling dim of $e = 1 - d/2 + m/4$

- e has positive scaling dimension at d_c for $1 < m < 2$

- $\Rightarrow$ cannot be the control parameter in perturbative loop expansions

- $e_{eff} = e^{\frac{2(m+1)}{3}} / \tilde{k}_F^{\frac{(m-1)(2-m)}{6}} \quad \left(\tilde{k}_F = k_F / \Lambda \right)$

has scaling dimension $[m + 3/(m+1) - d] (m+1)/3$ that vanishes at d_c

- $\Rightarrow$ effective coupling that is control parameter in loop expansions

One-Loop Results

Effective coupling
control parameter
in
loop expansions

$$\longrightarrow e_{eff} = e^{\frac{2(m+1)}{3}} / \tilde{k}_F^{\frac{(m-1)(2-m)}{6}}$$

Fixed points
of beta-function

$$\longrightarrow \tilde{\beta} \equiv \frac{\partial e_{eff}}{\partial \ln \mu} = \frac{(m+1)(u_1 e_{eff} - N\epsilon) e_{eff}}{3N - (m+1)u_1 e_{eff}} = 0$$

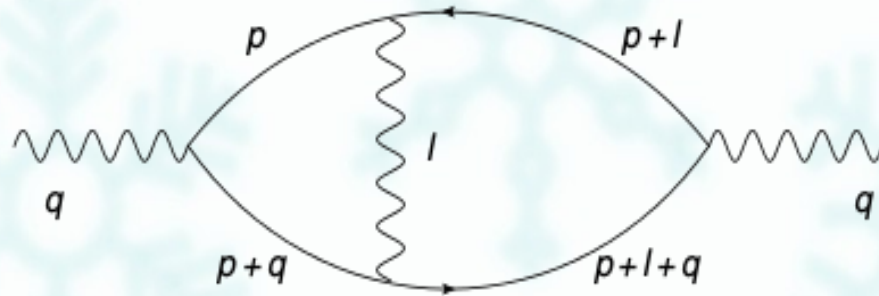
Interacting Fixed Point

$$\begin{aligned} e_{eff}^* &= \frac{N\epsilon}{u_1} \\ z^* &= 1 + \frac{(m+1)\epsilon}{3} \\ \eta_\psi^* &= \eta_\phi^* = -\frac{\epsilon}{2} \end{aligned}$$

Dynamical critical exponent

Anomalous dimensions for
fermions & boson

Two-Loop Boson Self-Energy



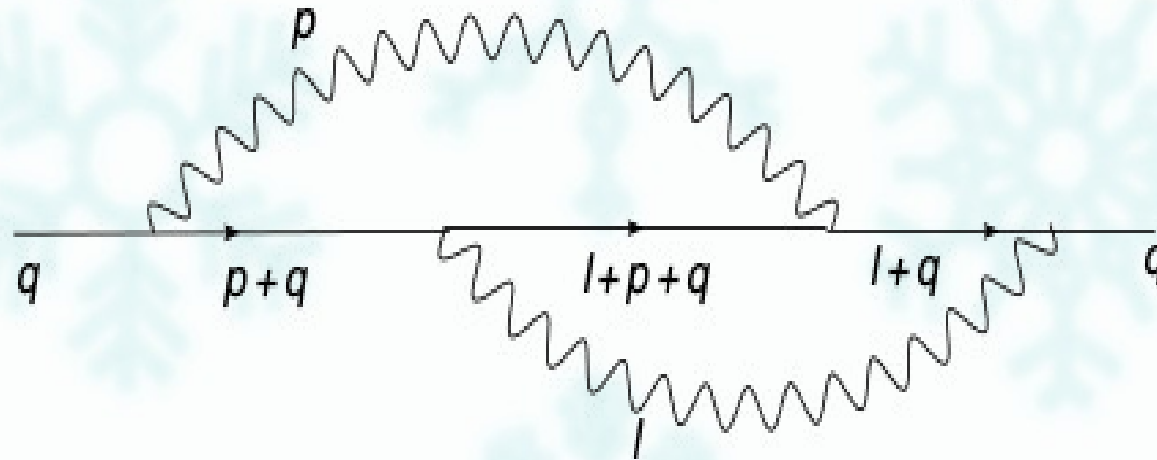
- For $m > 1$ • k_F suppressed • no correction

$$\Pi_2(q) \sim \frac{e^2 k_F^{\frac{m-1}{2}} \pi^2}{6 N |\vec{L}_{(q)}|^2 \sin\left(\frac{m\pi}{3}\right)} \frac{e_{eff}^{\frac{m}{m+1}}}{k_F^{\frac{m-1}{2(m+1)}}}$$

- For $m = 1$ • UV-finite correction

$$\Pi_2(q) \sim \left(\frac{e^2}{N |L_{(q)}|} \right) e_{eff}$$

Two-Loop Fermion Self-Energy



- For $m > 1$ ➡ $\Sigma_2(q) \sim k_F$ — suppressed

- ➡ no correction

- For $m = 1$ ➡ UV-divergent

Pairing Instabilities of Critical FS

FL unstable to arbitrary weak -ve interaction
in BCS channel leading to Cooper pairs
☞ How about a critical FS ?

[**IM**, *Phys. Rev. B* 94, 115138 (2016)]

Superconducting Instability

Add relevant 4-fermion terms

For simplicity, we consider s-wave case with 2 flavours

coupling constant

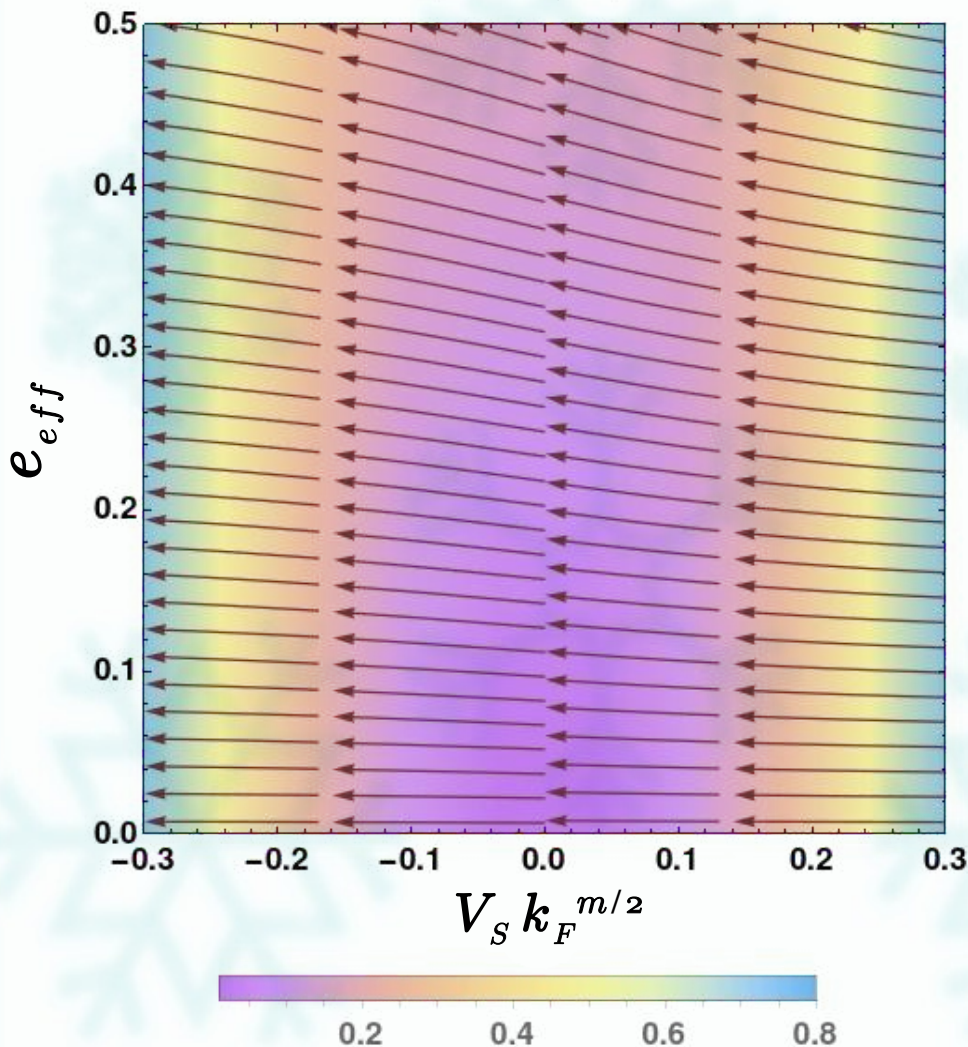
$$S^{\text{sc}} = \frac{\mu^{d_v} V_S}{4} \sum_{j_1, j_2} \int \left(\prod_{s=1}^4 dp_s \right) (2\pi)^{d+1} \delta^{(d+1)}(p_1 + p_2 - p_3 - p_4) (\delta_{j_1, j_2} - 1) \\ \times \left[\{ \bar{\Psi}_{j_1}(p_3) \Psi_{j_2}(p_1) \} \{ \bar{\Psi}_{j_2}(p_4) \Psi_{j_1}(p_2) \} - \{ \bar{\Psi}_{j_1}(p_3) \sigma_z \Psi_{j_2}(p_1) \} \{ \bar{\Psi}_{j_2}(p_4) \sigma_z \Psi_{j_2}(p_1) \} \right]$$

Coupled Beta-Functions for V_S & e_{eff}

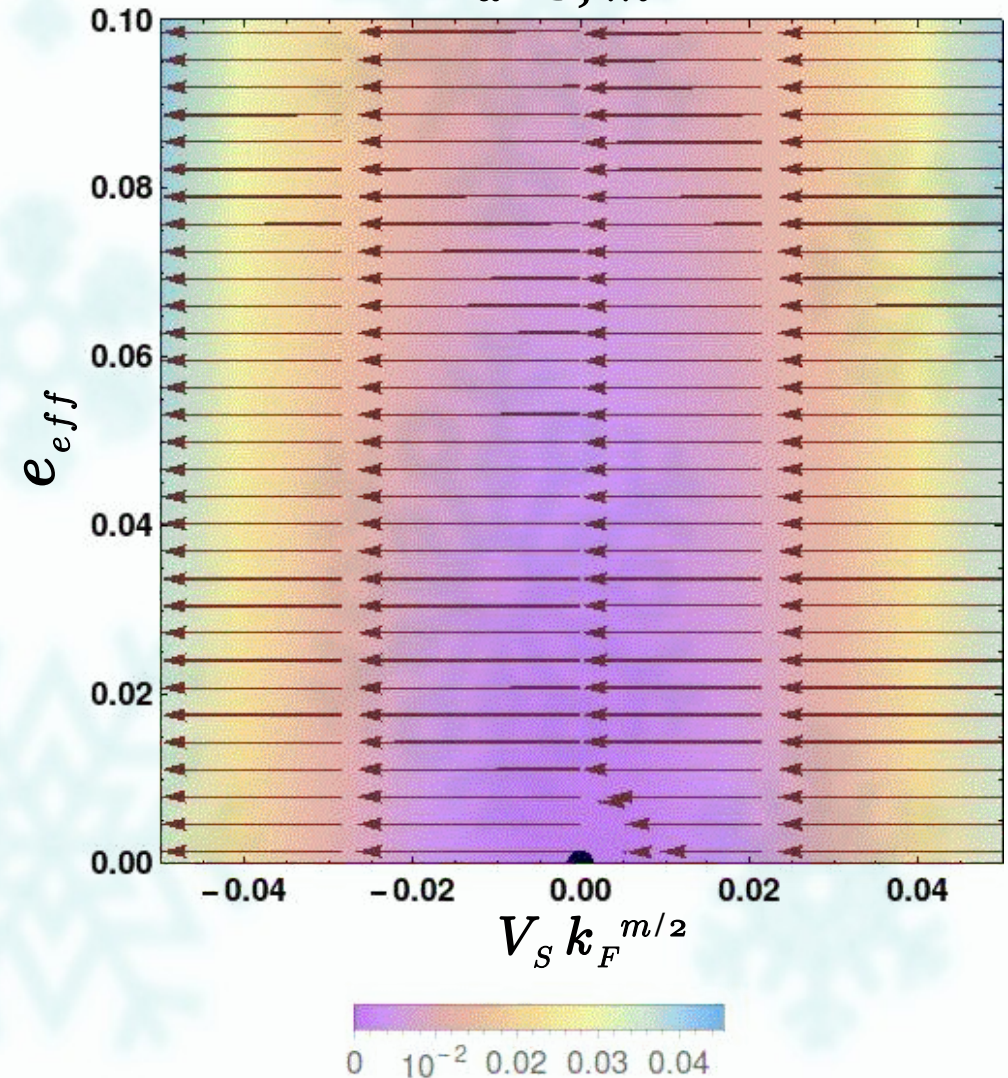
RG flows to $V_S \rightarrow -\infty$ for any initial V_S

↪ More susceptible to pairing than FL ($e_{\text{eff}} = 0$)

$d=2, m=1$



$d=3, m=2$



Fermi Surface
+
Transverse Gauge Field(s)

Fermi Surface + U(1) Gauge Field

$$\begin{aligned} S = & \sum_j \int \frac{d^{d+1}k}{(2\pi)^{d+1}} \bar{\Psi}_j(k) i \left[\mathbf{\Gamma} \cdot \mathbf{K} + \gamma_{d-m} \delta_k \right] \Psi_j(k) \\ & + \frac{1}{2} \int \frac{d^{d+1}k}{(2\pi)^{d+1}} \mathbf{L}_{(k)}^2 \phi(-k) \phi(k) \\ & + \frac{e}{\sqrt{N}} \sum_j \int \frac{d^{d+1}k d^{d+1}q}{(2\pi)^{2d+2}} \phi(q) \bar{\Psi}_j(k+q) \gamma_0 \Psi_j(k) \end{aligned}$$



Interaction vertex contains
 γ_0 instead of $i \gamma_{d-m}$

Values of $\mathbf{d}_c$ & critical exponents same as Ising-nematic case

[**IM**, *Phys. Rev. Research* 2, 043277 (2020)]

2 Fermion Flavours + $U_c(1) \times U_s(1)$

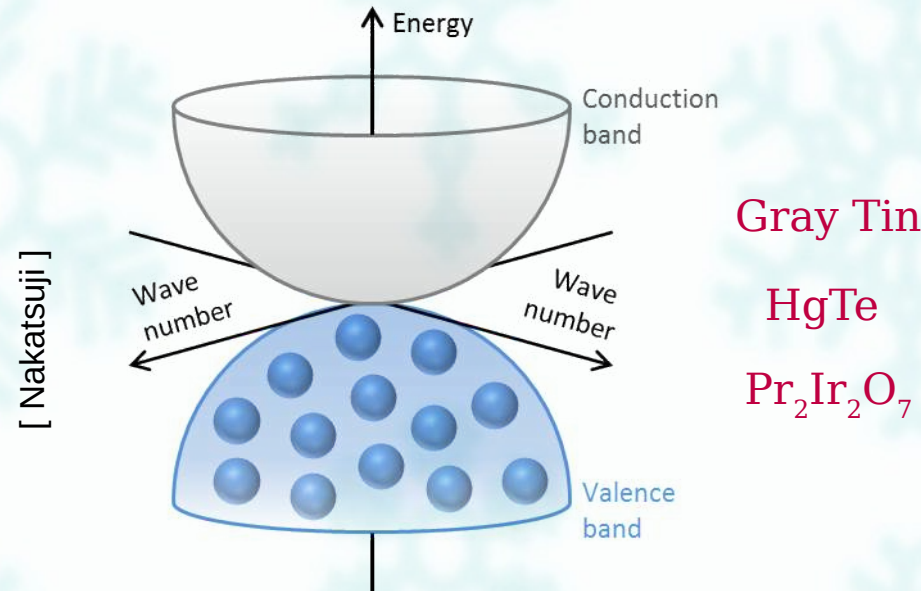
Model for QCPs for Mott insulator to metal & metal to metal transitions

[L. Zou & D. Chowdhury, *Phys. Rev. Research* 2, 023344 (2020)]

- First fermion couples to the gauge fields a_c & a_s as $(e^c a_c + e^s a_s)$
- Second fermion couples as $(e^c a_c - e^s a_s)$
- At one-loop, beta functions for the effective coupling constants give a **fixed line** $(e^c_{\text{eff}} + e^s_{\text{eff}}) \propto \epsilon$
- $m > 1$ ➡ fixed line feature survives at generic loops
[**IM**, *Phys. Rev. Research* 2, 043277 (2020)]
- $m = 1$ ➡ fixed line feature breaks at three-loop
[**IM**, *Phys. Rev. Research* 2, 043277 (2020)]

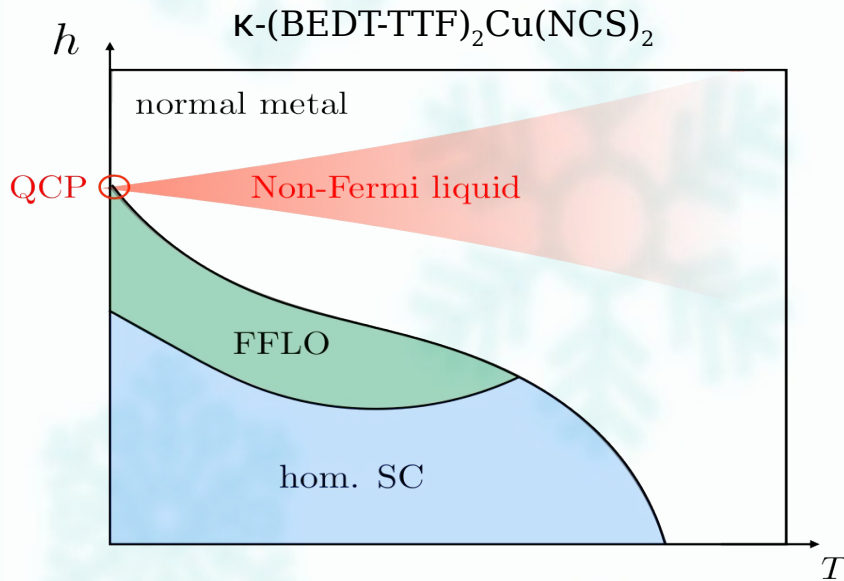
NFLs: Other Examples from My Work

Luttinger semimetals have quadratic band crossings



- Coulomb interactions drive it to NFL
 - Luttinger-Abrikosov-Beneslavskii phase
- NFL unstable to disorder
 - [R. M. Nandkishore & S. A. Parameswaran, *PRB* (2017); **IM** & R. M. Nandkishore, *PRB* (2018)]
- Optical, dc, thermal conductivities + thermoelectric coefficient computed
 - [**IM** & H. Freire, *PRB* (2021); H. Freire & **IM**, *Phys. Lett. A* (2021)]

NFLs: Other Examples from My Work

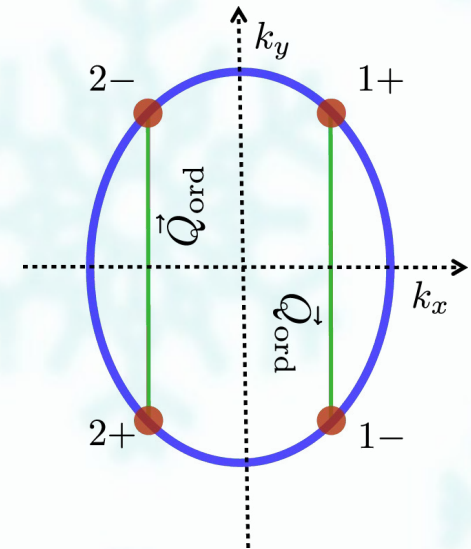


Fermi Surface

+

FFLO Boson

[D. Pimenov, **IM**, F. Piazza,
M. Punk, *PRB* (2018)]

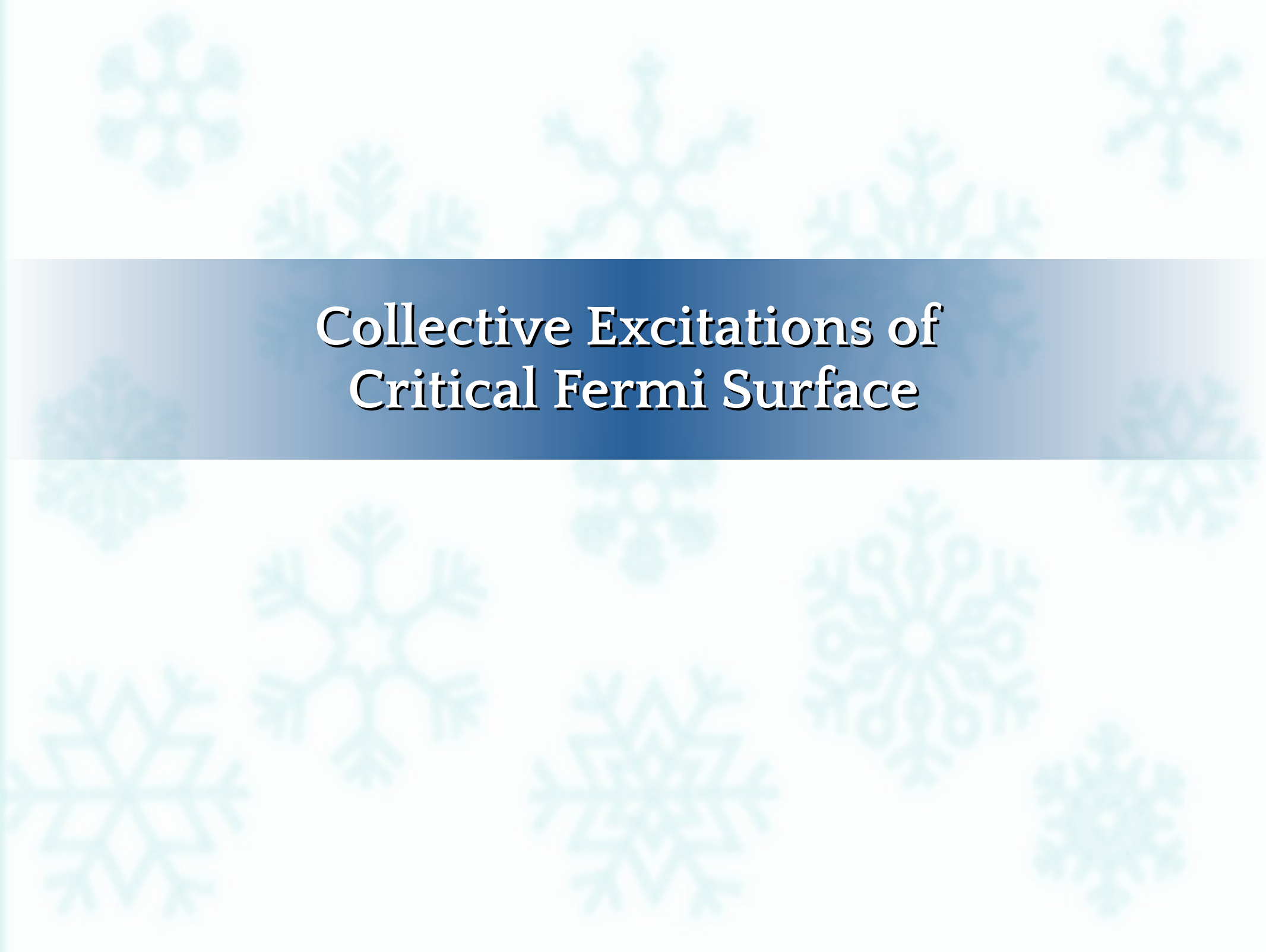


Fermi Surface

+

Spin Density Wave

[**IM**, *Ann. Phys.* (2015)]

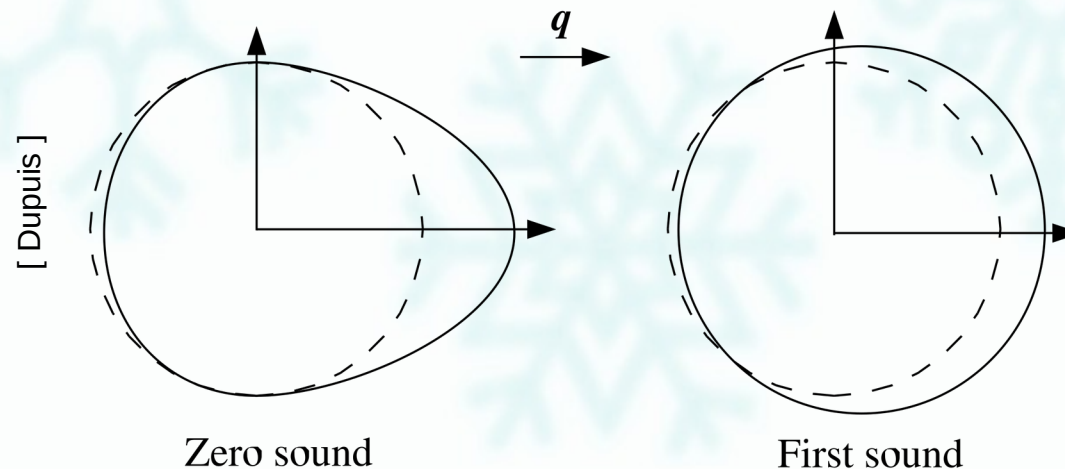


Collective Excitations of Critical Fermi Surface

Zero Sound for FL

Collective Mode in Collisionless Regime for Neutral FL

- Collective mode $\rightarrow$ density oscillation with wavevector q & frequency ν
- $\nu \gg$ Frequency of quasiparticle collisions ω
- Damping of zero sound from quasiparticle collisions negligible
- Excitations are localized close to the Fermi level
- Corresponds to an anisotropic redistribution of quasiparticles around the Fermi surface
- Transitions to first sound in the hydrodynamic regime ($\nu \ll \omega$)



Quantum Boltzmann Eqns (QBE)

Collective Mode in Collisionless Regime for Neutral FL

- FL $\rightarrow$ QBE of quasiparticles provides information about the low-energy excitations $\rightarrow$ E.O.M. of nonequilibrium Green's function
- Conventional derivation of the QBE relies on existence of quasiparticles:

spectral function

$$\xi_{\mathbf{k}} = \frac{k^2}{2m} - k_F, \quad A(\omega, \xi_{\mathbf{k}}, \theta_{\mathbf{k}}) = \frac{-2 \operatorname{Im} \Sigma^R(\omega, \xi_{\mathbf{k}})}{[\omega - \xi_{\mathbf{k}} - \operatorname{Re} \Sigma^R(\omega, \xi_{\mathbf{k}})]^2 + [\operatorname{Im} \Sigma^R(\omega, \xi_{\mathbf{k}})]^2}$$

$$\operatorname{Im} \Sigma^R \sim \omega^2 \ll |\omega| \text{ for } |\omega| \ll 1 \Rightarrow A \simeq 2\pi \delta(\omega - \xi_{\mathbf{k}} - \operatorname{Re} \Sigma^R)$$

$$G_0^< = i f_0(\omega) A, \quad \delta f \equiv f(\omega, \theta_{\mathbf{k}}; t, \mathbf{r}) - f_0, \quad \delta u(\theta_{\mathbf{k}}; t, \mathbf{r}) \sim \int d\xi_{\mathbf{k}} \delta f$$

linearized QBE

Fermi surface deformation

- E.O.M. of δf or δu $\rightarrow$ fails for NFLs

QBE for NFLs

$$\text{Im } \Sigma^R \sim |\omega|^{2/3} \gg |\omega| \text{ for } |\omega| \ll 1$$

- Spectral function A no longer a delta function
- f does not satisfy a closed E.O.M even at equilibrium
- Way out ☛ if self-energy is function of ω only, A is a sharply peaked function of ξ_k

Generalized distribution function

$$-i \int \frac{d\xi_{\mathbf{k}}}{2\pi} G^<(\omega, \xi_{\mathbf{k}}, \theta_{\mathbf{k}}; t, \mathbf{r}) \equiv f(\omega, \theta_{\mathbf{k}}; t, \mathbf{r})$$

[Prange & Kadanoff, 1964]

- E.O.M. of generalized Fermi surface deformation

$$\delta u(\theta_{\mathbf{k}}; t, \mathbf{r}) = \int \frac{d\omega}{2\pi} \delta f(\omega, \theta_{\mathbf{k}}; t, \mathbf{r})$$
$$\delta u_{\ell} = \int \frac{d\theta}{2\pi} \delta u(\theta; t, \mathbf{r}) e^{i\ell\theta}$$

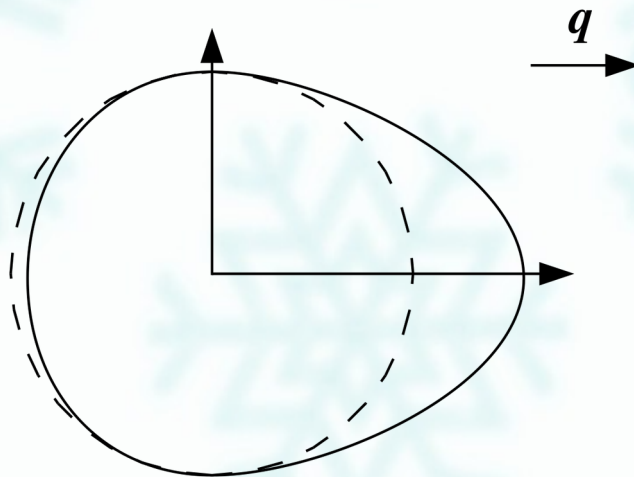
QBE for Ising-Nematic QCP

$$F_{Landau}(\omega_k, \theta) = e^2 m \operatorname{Re} \left[D_{1-loop}^R(\omega_k, |\theta|) \right] = \frac{e^2 m k_F^4 \theta^4}{k_F^6 \theta^6 + \frac{e^4 m^2 \omega_k^2}{\pi^2 v_F^2}}$$

$$\nu \delta u_\ell(\nu, \mathbf{q}) = v_F |\mathbf{q}| \frac{\delta u_{\ell+1}(\nu, \mathbf{q}) + \delta u_{\ell-1}(\nu, \mathbf{q})}{2 \left(1 + \frac{F_0 - F_\ell}{\pi} \right)}$$

Zero sound $\rightarrow \ell = 0$ channel

$$\nu = \frac{\pm \sqrt{2\pi} v_F |\mathbf{q}|}{\sqrt{\pi + 4 F_{01} - 2 F_{02} + \sqrt{4 F_{02}^2 + 12 \pi F_{02} - 8 \pi F_{01} + \pi^2}}}$$



Zero sound

Charged NFL: Plasmons

$$(\nu + i \gamma \delta_{|\ell|>1}) \delta u_\ell(\nu, \mathbf{q}) = -\sigma_3 v_F |\mathbf{q}| \frac{\delta u_{\ell+1}(\nu, \mathbf{q}) + \delta u_{\ell-1}(\nu, \mathbf{q}) + F_c u_0 \delta_{|\ell|,1}}{2 \left(1 + \frac{F_0 - F_\ell}{\pi}\right)}$$

$$F_c = \frac{2 \pi \alpha}{\lambda_F |\mathbf{q}|}$$

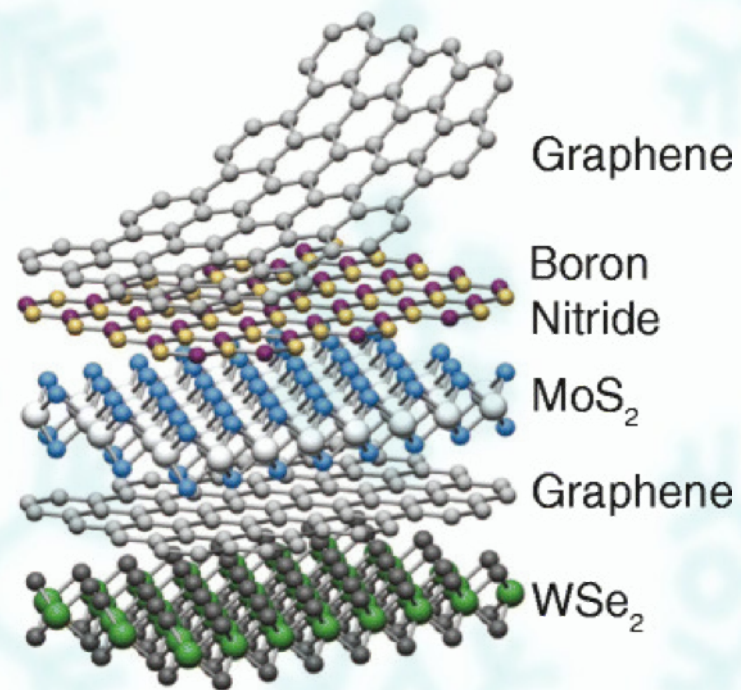
Coulomb via RPA

- Plasmon $\ell = 0$ channel, $\mathbf{q} \rightarrow 0$

$$\nu = \frac{\pm \pi v_F \sqrt{|\mathbf{q}|} \sqrt{\frac{2 \alpha}{\lambda_F}}}{\sqrt{\pi + 2 F_{01} - F_{02} + \sqrt{(F_{02} + \pi)^2}}} - i \gamma \frac{\lambda_F |\mathbf{q}|}{8 \pi \alpha}$$

- Transitions to zero sound of neutral NFL for larger $\mathbf{q}$

Moiré Superlattices

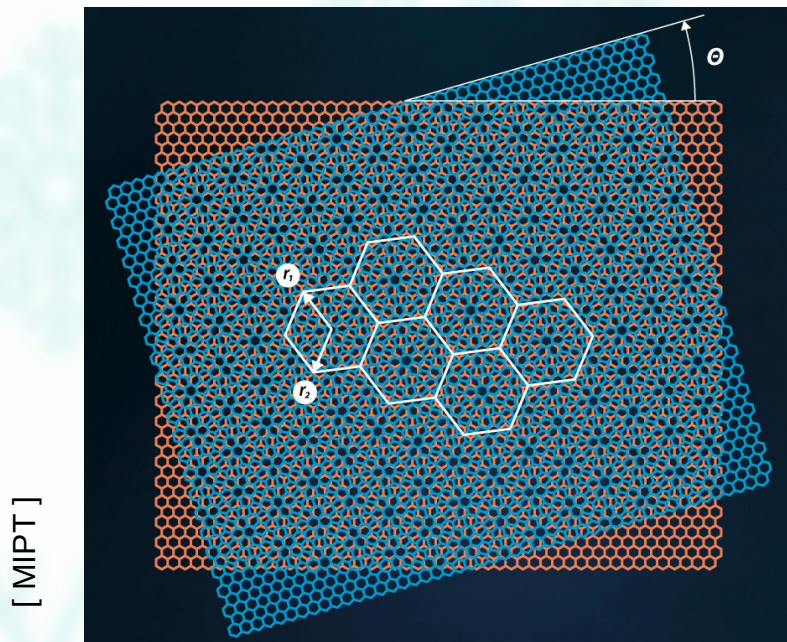


[Geim]

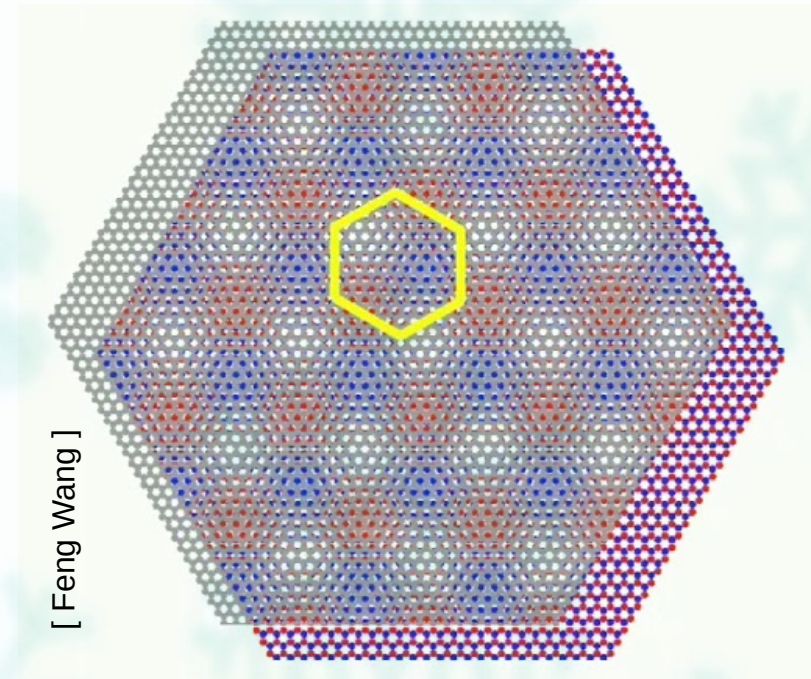
Moiré Superlattices

2 or more atomically-thin sheets of periodic patterns overlaid with a relative twist or a mismatched lattice constant
☞ **(Quasi)-periodic interference pattern**

Twisted Bilayer Graphene



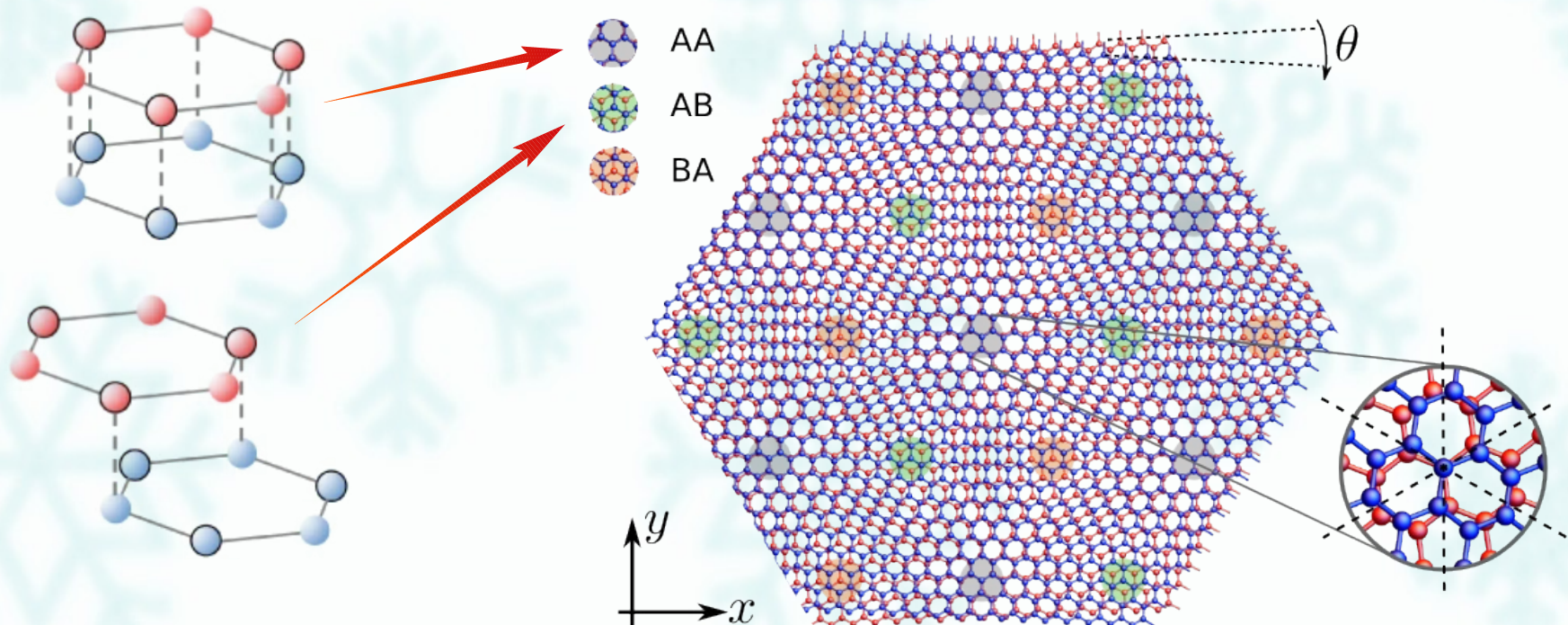
Aligned Graphene-hBN



- ▶ Experimentally realized by stacking 2D materials
- ▶ Enlarged unit cell

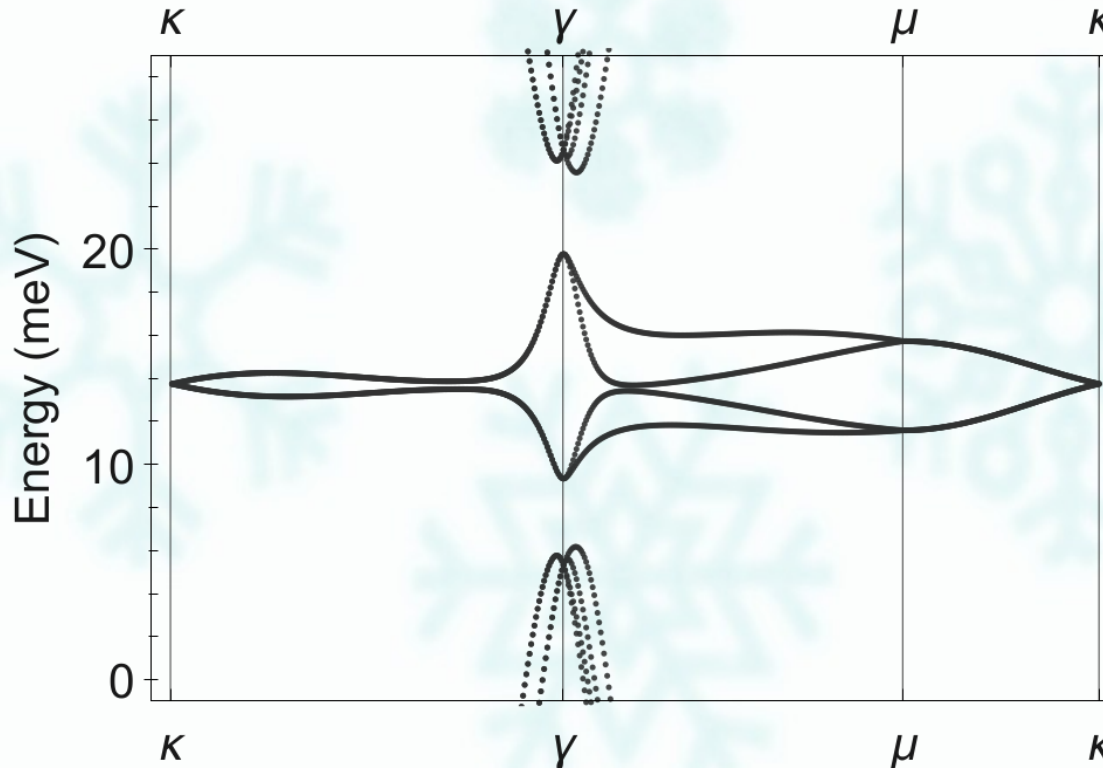
Magic-Angle Twisted Bilayer Graphene

- ▶ For small twist-angles $\theta \sim 1^\circ$
 - ☛ large moiré unit cell $\sim 10^4$ atoms (10 nm)
- ▶ 3 notable regions: AA, AB, BA, each forming a triangular lattice
- ▶ AB and BA sites together form a honeycomb lattice
- ▶ Show insulating behavior when moiré bands are partially filled



Platform for Strong Correlations

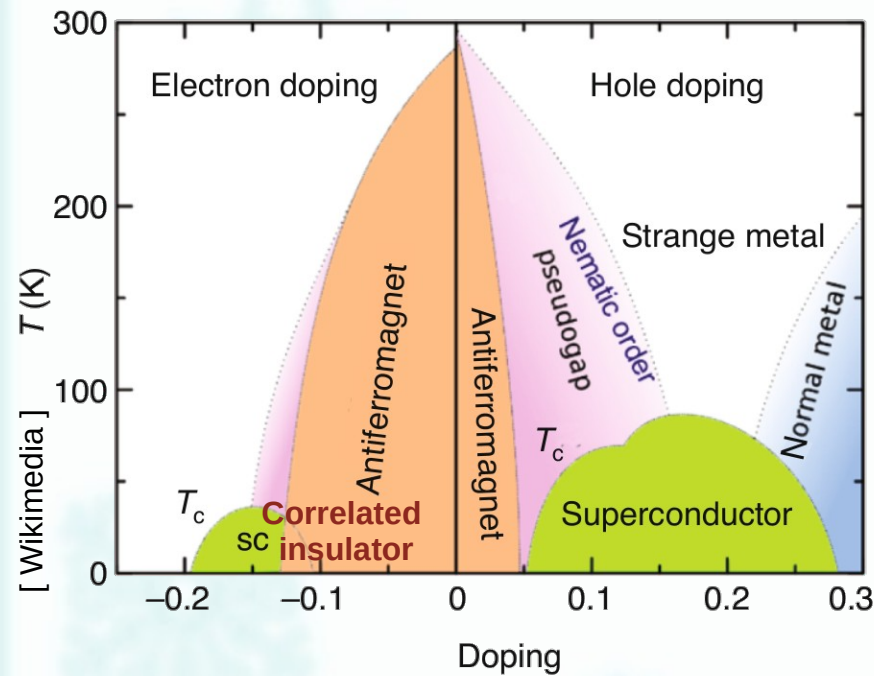
- ▶ Moire periodicity $\gg$ larger than either lattice constant
- ▶ Increase in lattice length $\Rightarrow$ electron propagates at a longer wave length on the lattice $\Rightarrow$ lower momentum / reduced K.E.
- ▶ Interaction energy $\gg$ K.E.
- ▶ Magic angles $\Rightarrow$ bands near charge neutrality become nearly flat



[Black-Schaffer et al (2021)]

Low energy band structure of TBG at $\theta \approx 1.2^\circ$

Moiré: Simpler + Highly Tunable



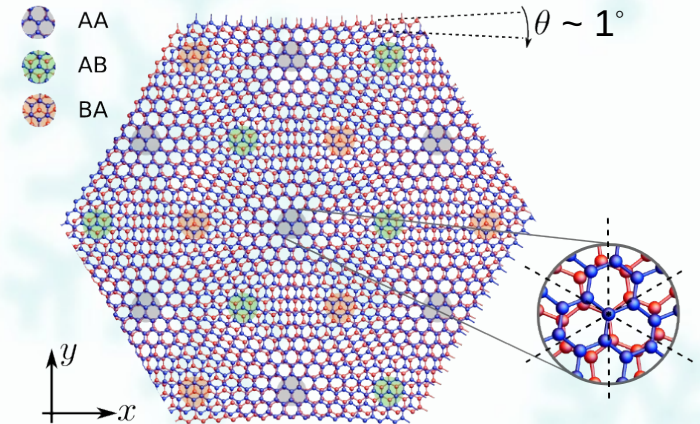
Phase diagram of cuprates



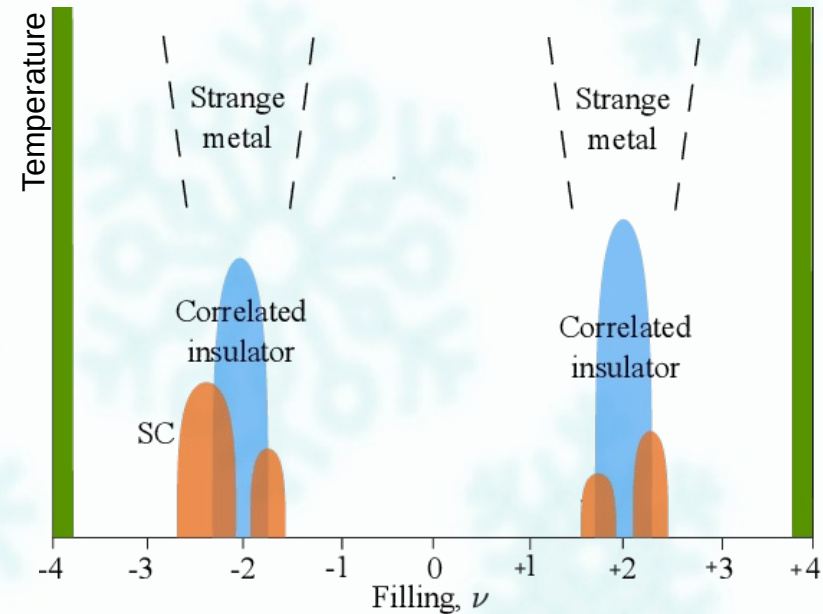
New insights into
high- T_c
&
strange metals?

**Chemical complexity
replaced by
structural complexity**

Magic-Angle Twisted Bilayer Graphene



[Thomson et al (2018)]

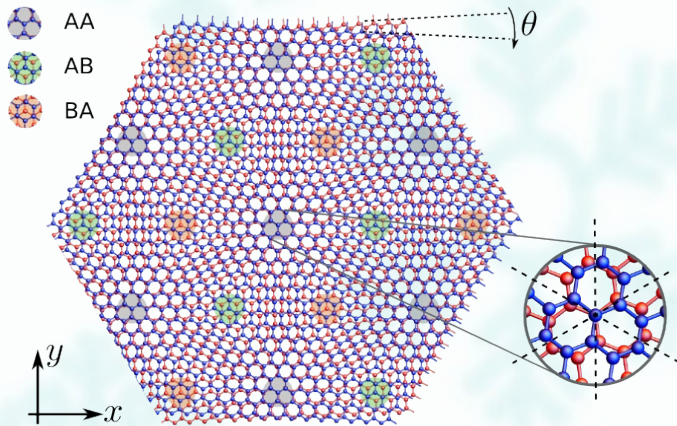


Correlated insulators at half-fillings

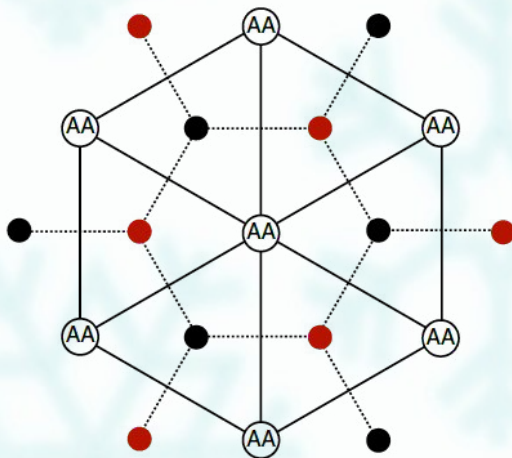
[Cao et al (2019)]

Moiré: My Recent Work

Magic-Angle Twisted Bilayer Graphene

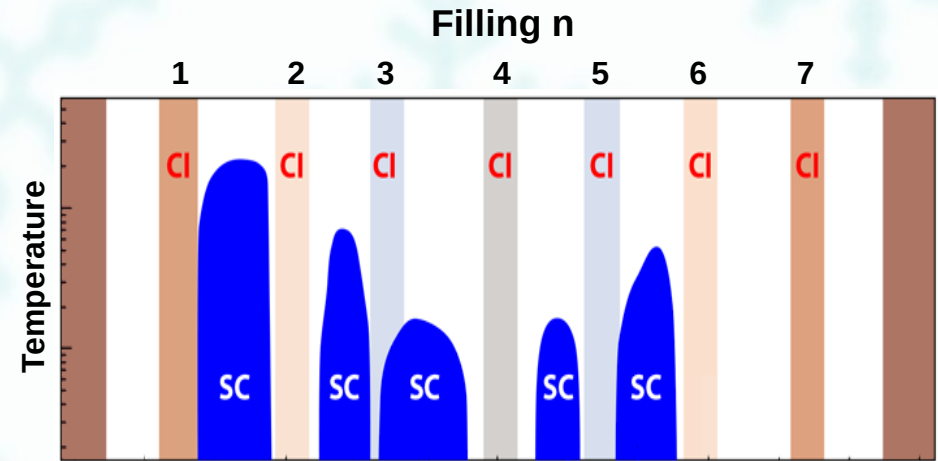


Thomson et al (2018)



8 states per moiré unit cell:

2 (spin) x 2 (sublattice) x 2 (valley)



MacDonald (2019)

Correlated insulators (**CI**)

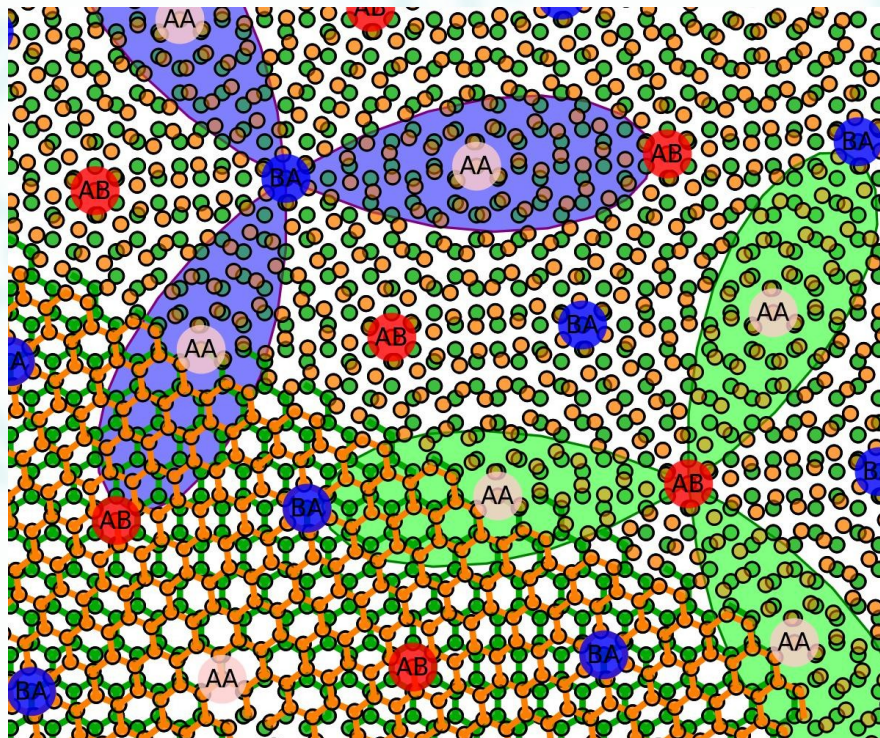
at integer fillings

[**IM**, J. Yao, E. J. Mueller,
PRB (2021)]

**Identify static charge
configurations**

A Simple Model

- ▶ Full lattice model is challenging $\sim 10^4$ bands
- ▶ Electronic structure of low-energy bands built from Wannier orbitals centered at AB & BA sites
- ▶ Each Wannier state has a 3-lobed spatial structure ➡ each lobe centered on an AA site [Koshino et al, Phys. Rev. X 8, 031087 (2018)]
- ▶ In addition to sublattice index (AB or BA), Wannier states labelled by spin and valley indices ➡ 8-band effective Hamiltonian



Subtleties

- ▶ There is a topological obstruction that prevents the existence of exponentially localized Wannier states obeying all the emergent symmetries
- ▶ Wannier states that we work with are exponentially localized, with one of the protecting symmetries broken
- ▶ These considerations only affect physics on an exponentially small energy scale: irrelevant to the questions we are asking

[Wang and Vafek, *PRB* (2020)]

Energy Scales

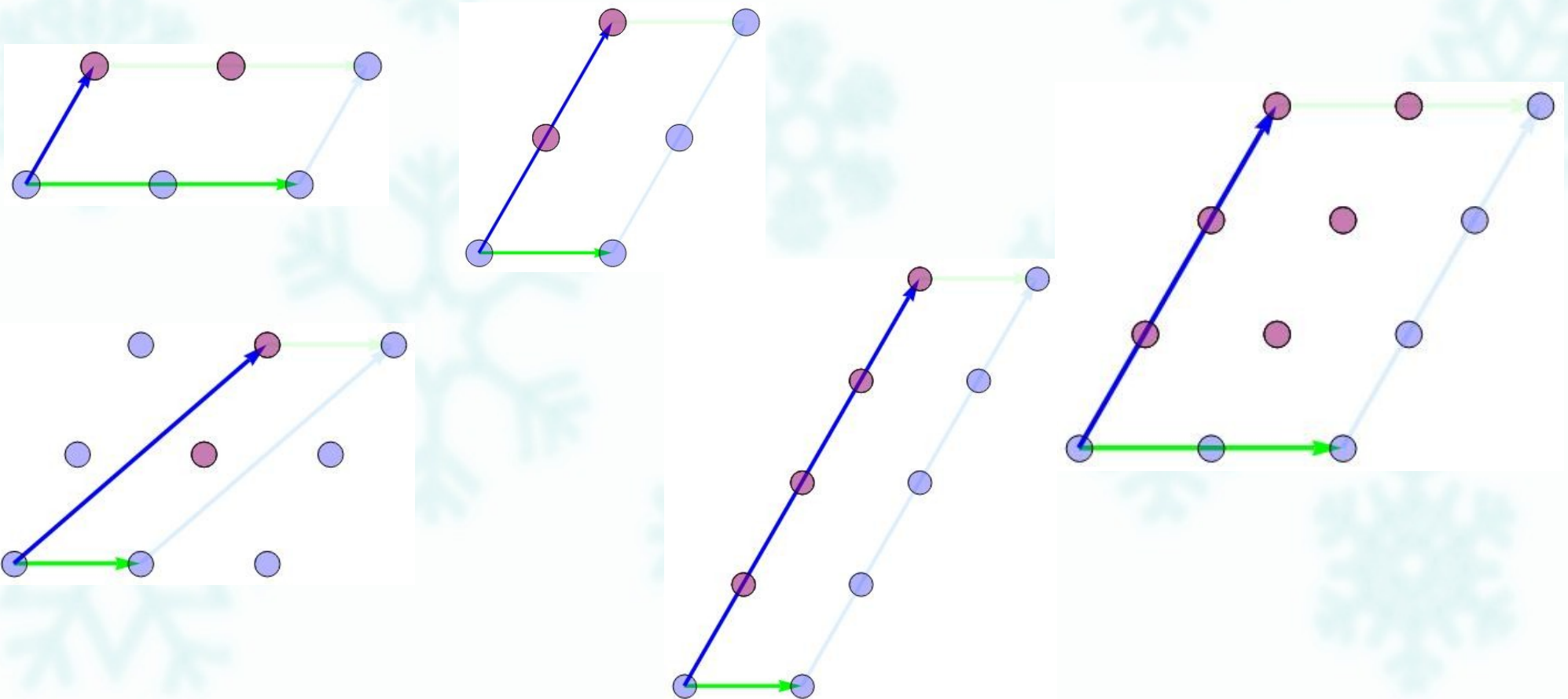
- ▶ Effective electronic hopping matrix element between two nearest Wannier orbitals ~ 0.3 meV
- ▶ Effective direct Coulomb interaction between them ~ 10 meV

[Koshino et al, *PRX* (2018)]

- ▶ We neglect kinetic energy and find stationary charge configurations which minimize the Coulomb interaction energy

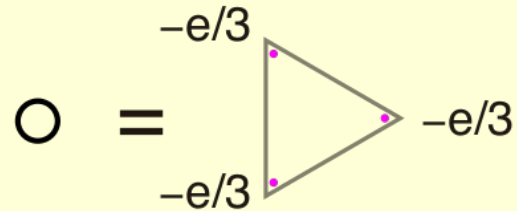
Procedure

- ▶ Consider periodic arrangements of charges defined by the generators $\mathbf{v}_1 = m_1 \mathbf{a}_1 + m_2 \mathbf{a}_2$ and $\mathbf{v}_2 = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2$
- ▶ We include all unit cells containing fewer than 13 sublattice sites, with $m_1, m_2, n_1, n_2 \leq 4$
- ▶ In all, we consider well over 3000 charge configurations



Procedure ...

- For a single electron, each of the 3 lobes of a Wannier orbital accommodates a charge of $-e/3$ (fracton)



- Coulomb interaction energy from the fractons well approximated by

$$V_{ij} = \begin{cases} \frac{e^2}{9 \epsilon L_M} \frac{1}{|r_i - r_j|} & r_i \neq r_j \\ \frac{e^2}{9 \times 0.28 L_M} & r_i = r_j \end{cases}$$

for two fractons located at the same lobe

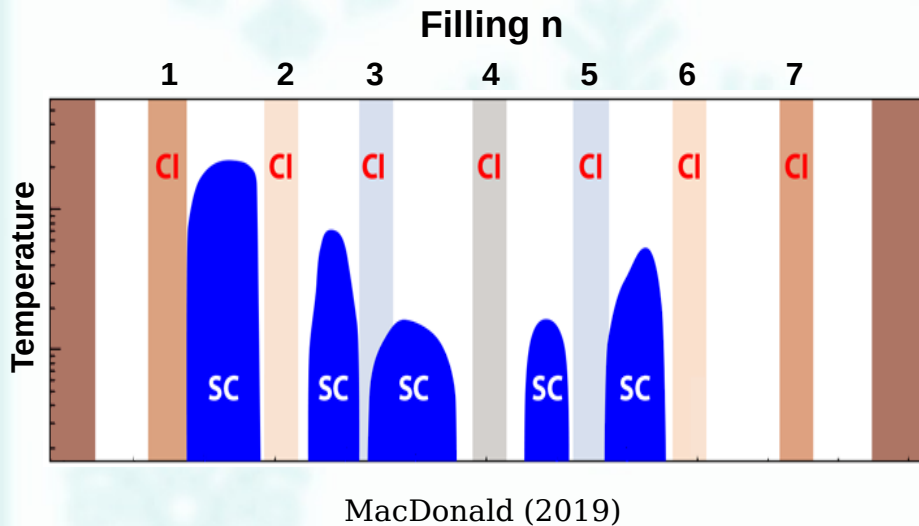
- We include exchange interaction that lowers energy by J when two overlapping occupied orbitals have same spin and valley quantum numbers (Hund's rule)

Procedure ...

- ▶ Coulomb interaction energy from a 2D array of charges is linearly divergent with system size
- ▶ The relative energies of the configurations with the same average density, however, are well defined
- ▶ After subtracting off the leading divergence, the remaining sums regularized by using 2D Ewald sums

Moiré: My Recent Work

Magic-Angle Twisted Bilayer Graphene



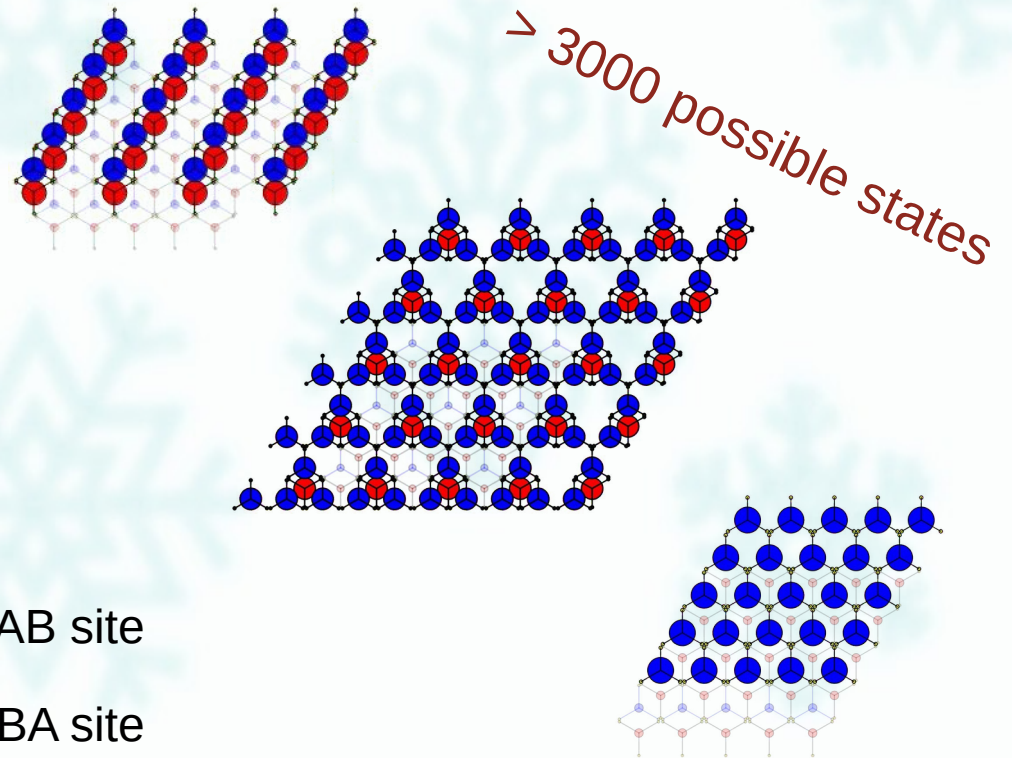
Correlated insulators (**CI**)
at integer fillings
of 8 moiré bands

[IM, J. Yao, E. J. Mueller,
PRB (2021)]

Identify static charge
configurations

E.g. $n = 1$

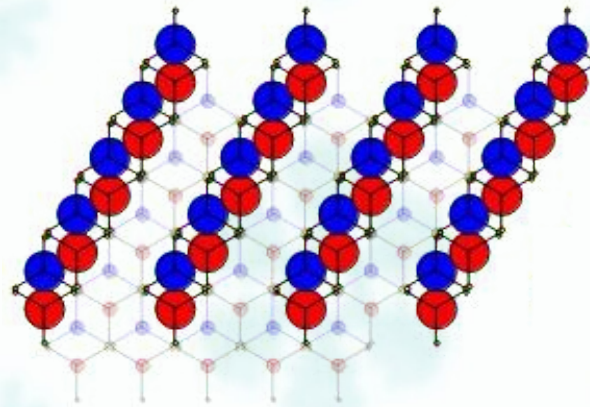
Which one
has lowest
energy?



Ground States

Energy minimization

Striped
Ferromagnet
☛ Ground State
at $n = 1$



[**IM**, J. Yao, E. J. Mueller,
PRB (2021)]

Agrees with
experiments

[Zondiner et al, *Nature* (2020)]

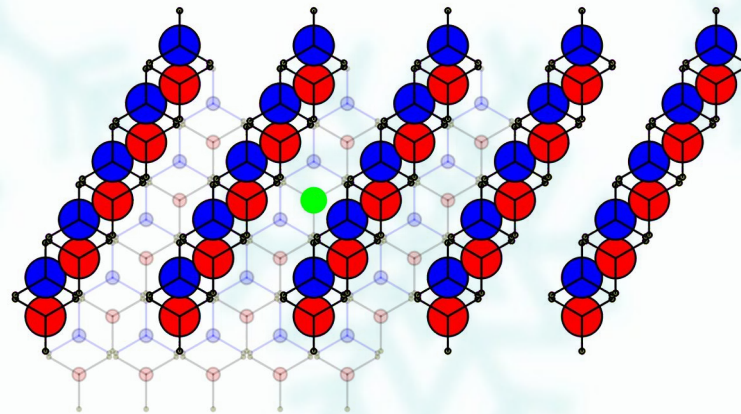
[Choi et al, *Nature* (2019)]

[Lu et al, *Nature* (2019)]

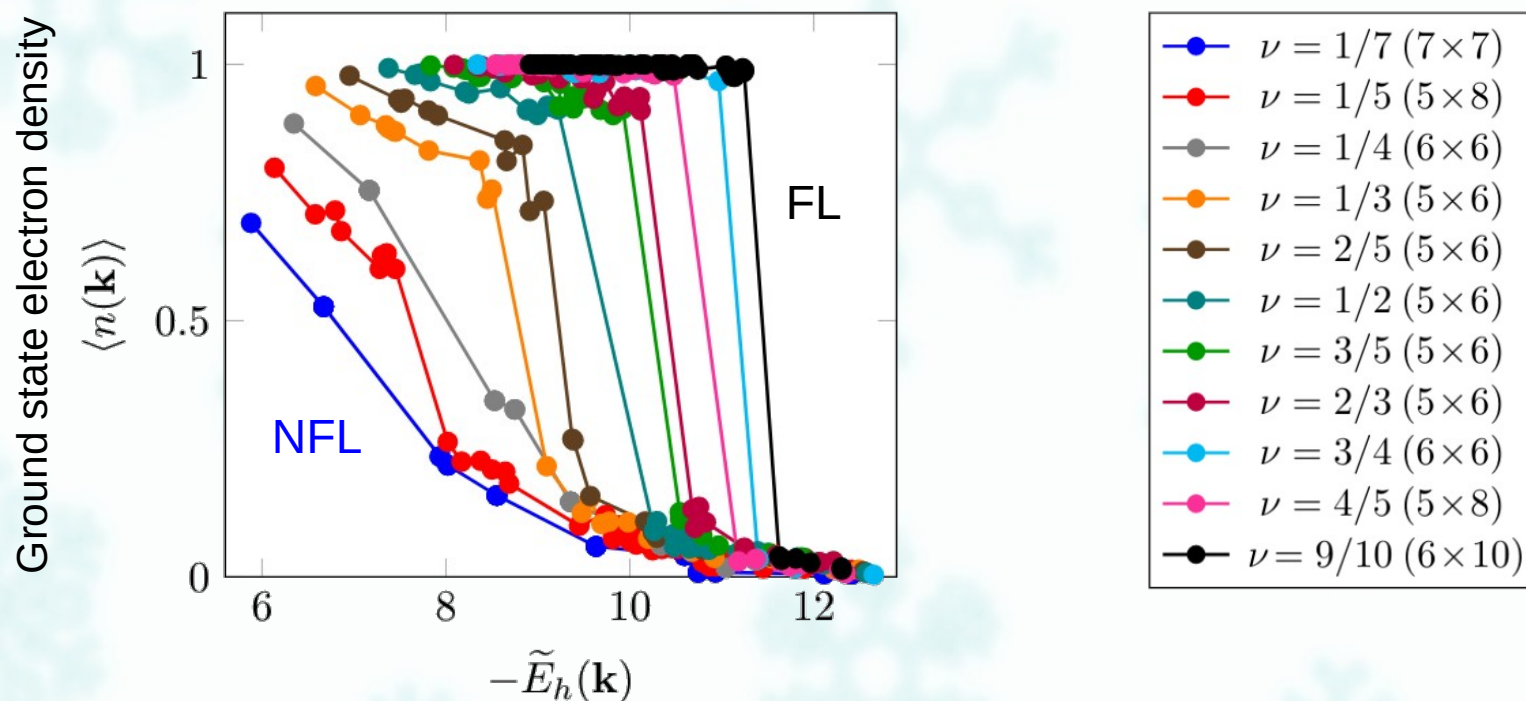
Excitations

Energy of 4 types of excitations:

- ▶ adding a single electron
- ▶ removing a single electron
- ▶ creating an electron-hole pair
- ▶ flipping spin / valley of a single electron



Current + Future Plan



[A. Abouelkomsan, Z. Liu, & E. J. Bergholtz, *PRL* (2020)]

Interaction-driven FL / NFL in ABC-stacked trilayer graphene
at fractional fillings ν

- Identify possible ordering instabilities
- Compute free energy to find the ground states
- Construct a field theory action to derive RG equations

International Collaborations

Yukawa-SYK Models

Yuxuan Wang
University of Florida

Superconductivity mediated by antiferromagnetic magnons

Akashdeep Kamra
IFIMAC, Universidad Autónoma de Madrid

Transport in 2d / 3d structures

Klaus Zeigler
Universität Augsburg

Order parameters in moiré lattices

Rafael M. Fernandes
Uni. of Minnesota

Fractionally-filled moiré flat-bands

Emil J. Bergholtz
Stockholm Uni.

Twisted Bilayer Cuprates

Annica Black-Schaffer
Uppsala Uni.

and others....

Thank you for your attention!

54 Papers

16 single auth.

16 major collabs.

Quantum Condensed Matter
with a focus on
Strongly Correlated Systems

Strange Metals
or
Non-Fermi liquids

2d multi-layers
☛ **Moiré superlattices**

Procedure ...

- ▶ Coulomb interaction energy from a 2D array of charges is linearly divergent with system size
- ▶ The relative energies of the configurations with the same average density, however, are well defined
- ▶ After subtracting off the leading divergence, the remaining sums regularized by using 2D Ewald sums

$$\sum_{\mathbf{w} \in \mathcal{L}} \frac{1}{|\mathbf{r} - \mathbf{w}|} = f_s(\mathbf{r}) + f_l(\mathbf{r}) + C$$
$$f_s = \sum_{\mathbf{w} \in \mathcal{L}} \frac{1}{|\mathbf{r} - \mathbf{w}|} \operatorname{erfc} \left(\frac{|\mathbf{r} - \mathbf{w}|}{2\eta} \right) - \frac{4\sqrt{\pi}}{\Omega} \eta$$
$$f_l = \frac{2\pi}{\Omega} \sum_{\mathbf{k} \in \bar{\mathcal{L}} \setminus 0} \frac{e^{i\mathbf{k} \cdot \mathbf{r}}}{2k} \operatorname{erfc}(k\eta)$$

Sum is over a Bravais lattice generated by the supercell vectors $\mathbf{v}_1, \mathbf{v}_2$