Simulatable Models of Non-Fermi Liquids & Nodal Superconductors

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Superconductivity:

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Non-fermi liquids:

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Bimla Danu

Johannes Hoffman

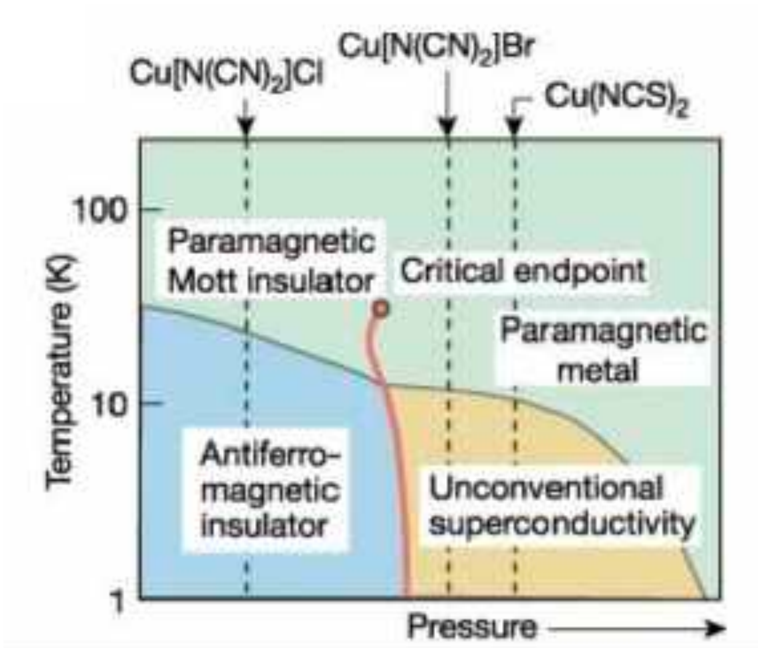
Matthias Vojta

Funding: NSF DMR-1752417, Sloan Research Fellowship.

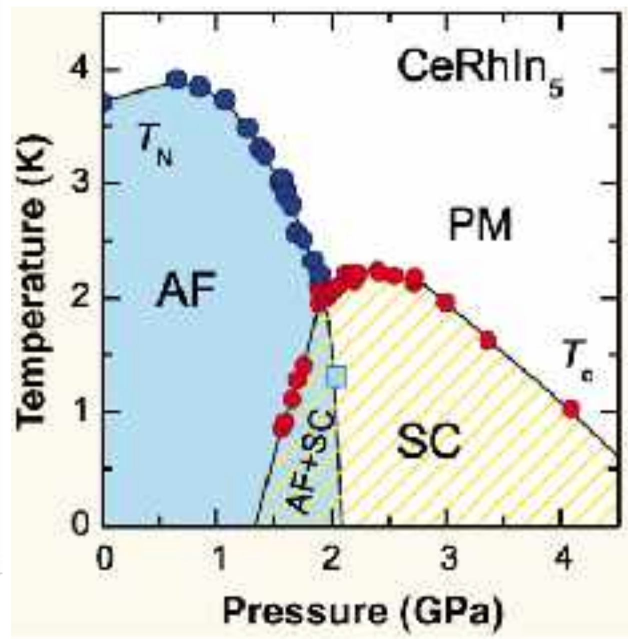
Outline

- Motivation
- The sign problem - picking your poison.
- Competing nodal superconductivity and AFM.
- Fractionalized Heavy fermi systems.

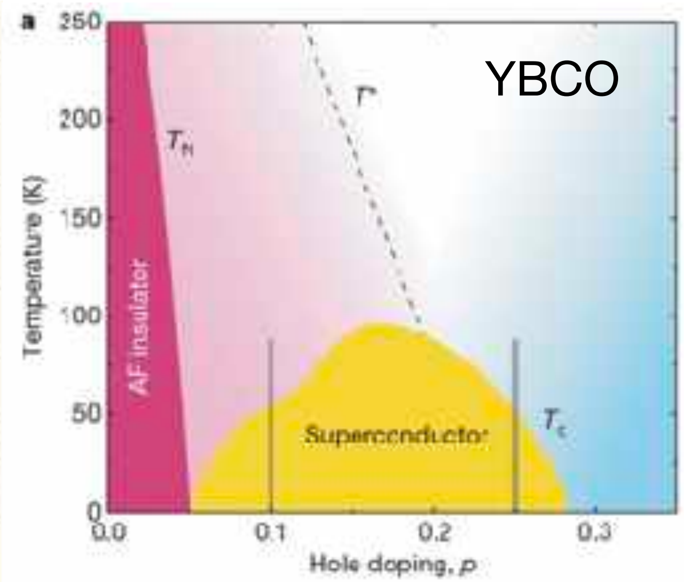
Motivation



[Kawaga et al 2005]



[Knebel et al 2009]

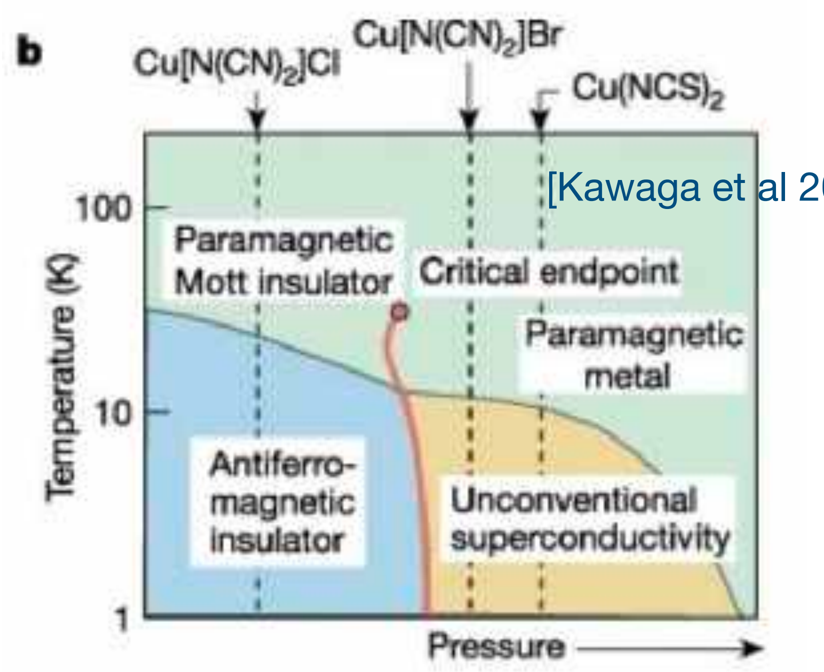


[Doiron-Leyraud et al 2007]

Solvable or simulatable models that capture

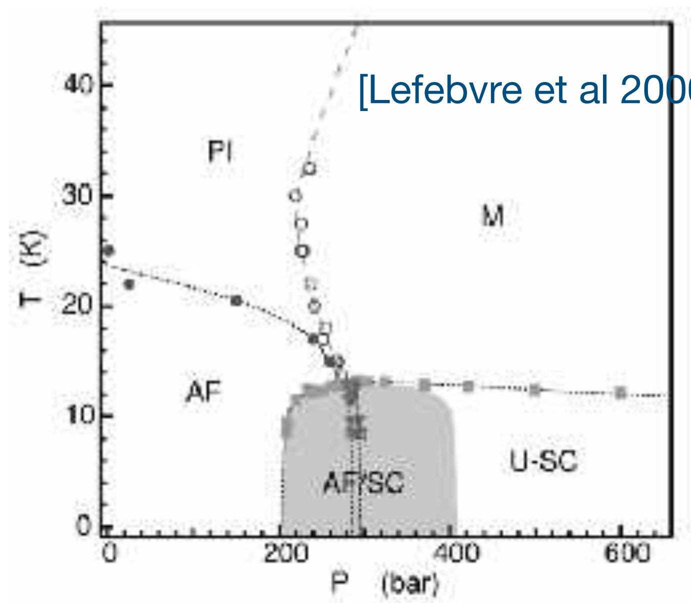
Mott physics, nodal-SC and AFM all together?

Not uncommon to find nodal SC close to pressure-tuned Mott transition…



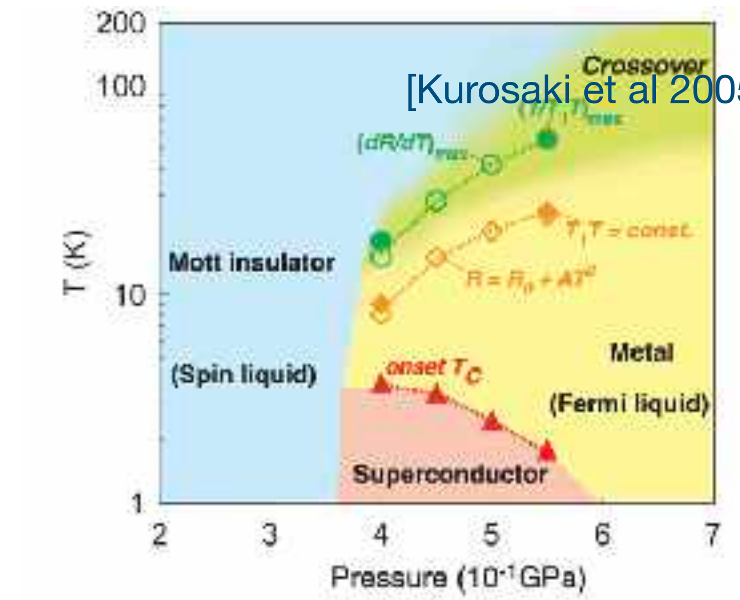
[Kawaga et al 2005]

Phase diag. of $\varkappa$-Cl

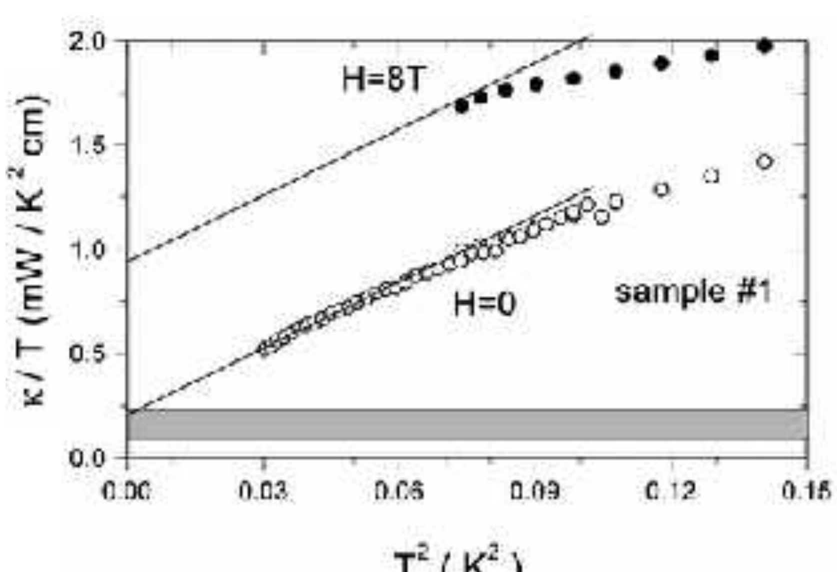


[Lefebvre et al 2000]

Phase diag. of $\varkappa$-(CN)$_3$

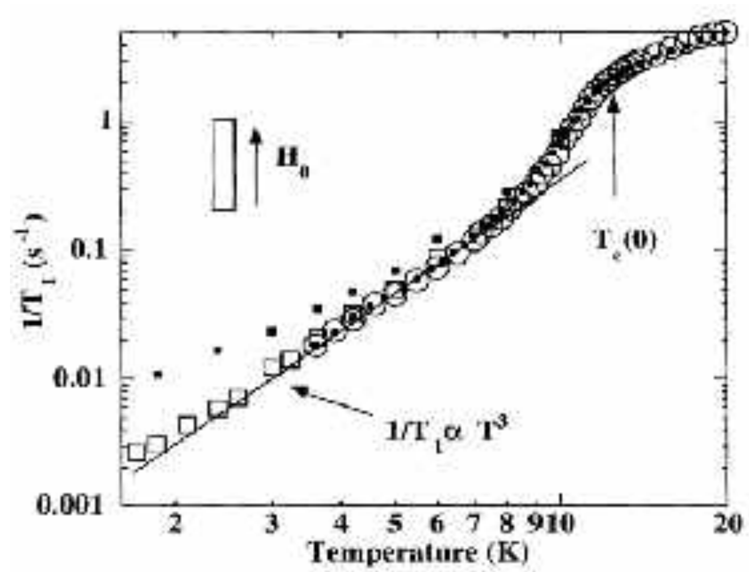


[Kurosaki et al 2005]



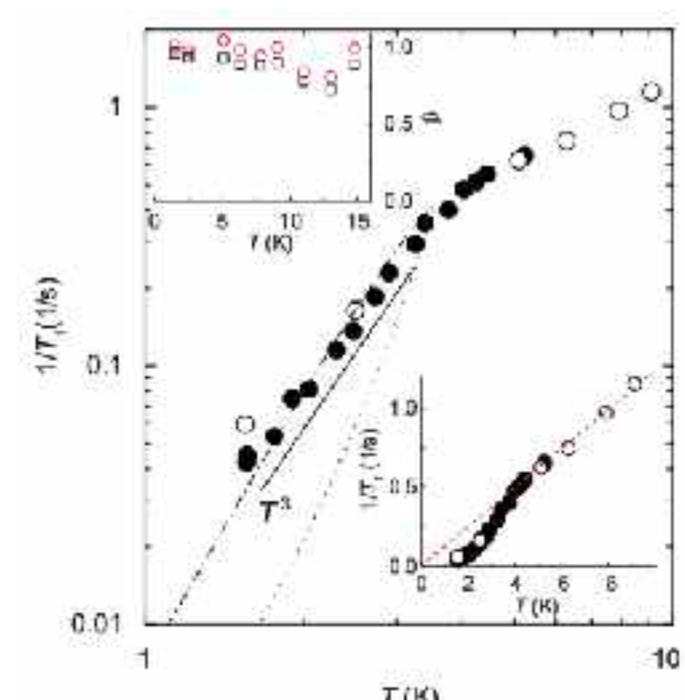
Thermal conductivity of $\varkappa$-(NCS)$_2$

[Belin et al 1998]



NMR 1/T$_1$ in $\varkappa$-Br

[Mayaffre et al 2000]

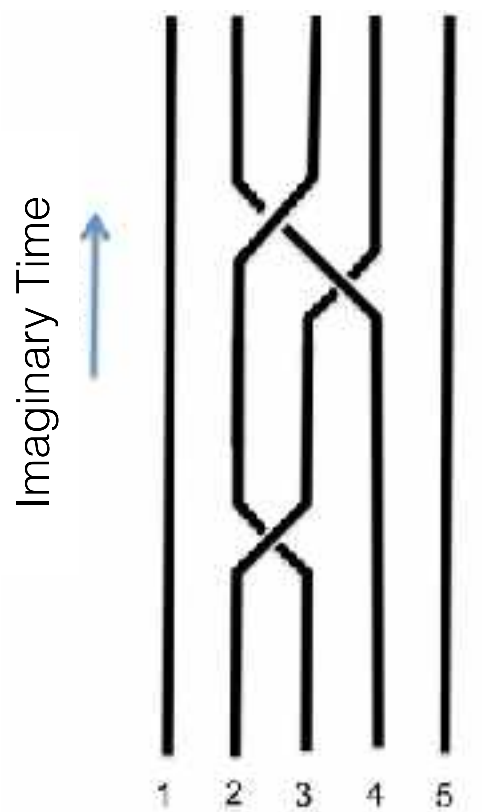


NMR 1/T$_1$ in $\varkappa$-(CN)$_3$

[Shimizu et al 2010]

Simulatable Models?

"Fermion sign problem": Repulsive onsite interactions ("Mottness")+ Fermi surface makes Monte Carlo impossible.



$$Z = \sum_{\{C\}} (-1)^{\text{\# of fermion exchanges in a configuration C}} |\text{Weight}(C)|$$

$$\sim 1 - 1 + 1 - 1 \ldots$$

“De-signer” models

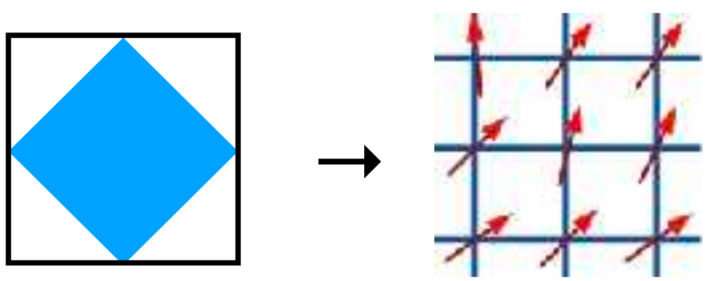
Pick your poison…

Want Mott Physics… Vs Want Fermi surfaces …

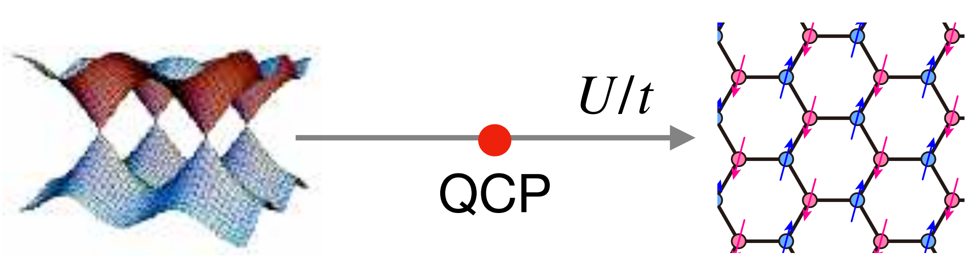
Main caveat:

Restricted to half-filling and bipartite lattices.

- Fermi surface nesting, leading to immediate AFM instability.



- Dirac semi-metal competing with AFM.



[Assaad, Herbut 2013; Otsuka et al 2016,…]

Typically (not always), multi-band Hubbard models with inter-band repulsion and intra-band onsite attraction.

[Wu, Zhang 2005]

Can capture some competing orders such as nematic, spin-density wave, non-nodal SC.

[Berg et al 2012; Schattner et al 2015; Dumitrescu et al 2016; Li et al 2017; Lederer et al 2017; Wang et al 2017, …]

Main caveat: no Mott physics, no nodal SC, s-wave SC can lurk at low-T which can obscure T = 0 QCP.

We will be interested in competing nodal SC and AFM.

Key observation: neither of these phases *require* any doping.

Can one find *any* simulatable model at all that hosts these phases?

Assaad, Imada, Scalapino (1996)

$$H = H_t + H_U - W \sum_{\langle i,j \rangle} (c^\dagger_{i,\sigma} c_{j,\sigma} + \text{h.c.})^2$$

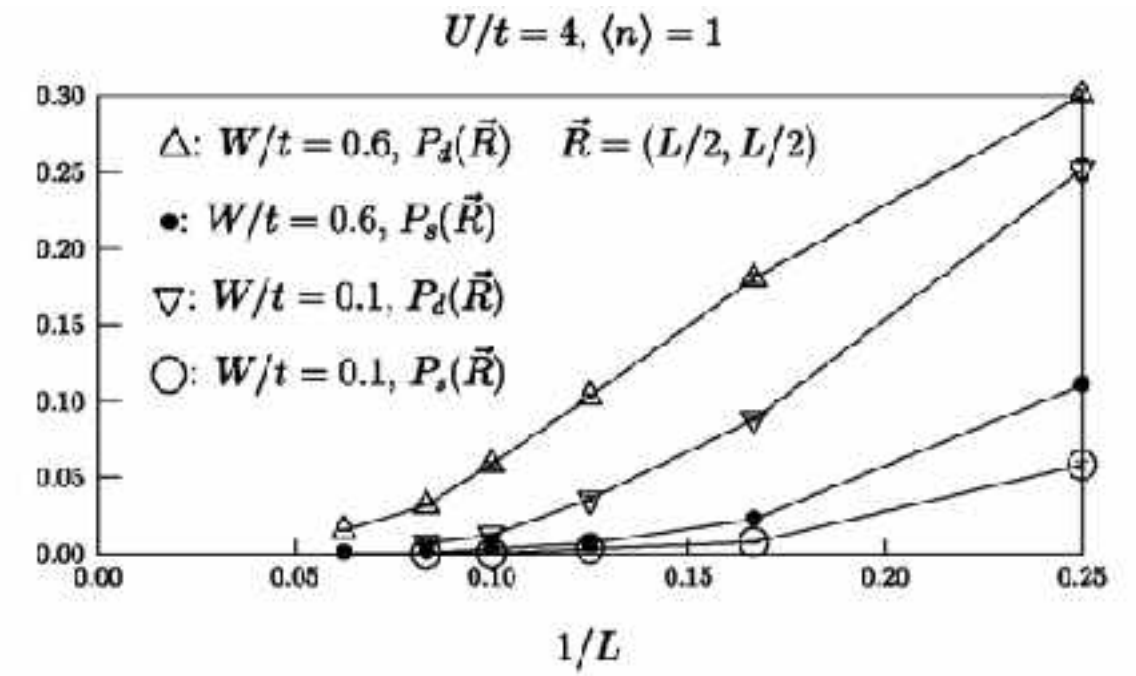


FIG. 2. $d_{x^2-y^2}$ (triangles) and s-wave (circles) pair-field correlations versus $1/L$.

We will be interested in competing nodal SC and AFM.

Key observation: neither of these phases *require* any doping.

Can one find *any* simulatable model at all that hosts these phases?

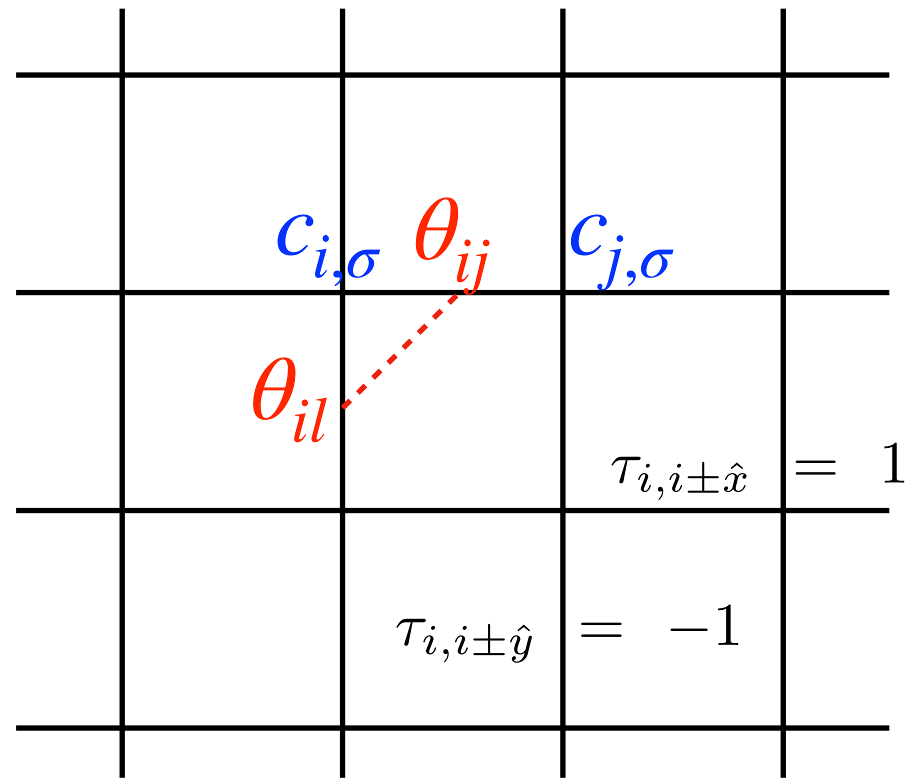
Here we will introduce a new model that demonstrably
hosts both nodal d-wave SC and AFM phases.

The model

$$H = H_t + H_U + H_V + H_{XY}$$

$$H_{\rm XY} = K\sum_{\langle ij\rangle} n_{ij}^2 - J\sum_{\langle ij,il\rangle}\cos(\theta_{ij}-\theta_{il})$$

$$H_V = V\sum_{\langle ij\rangle}(\tau_{i,j}e^{\mathrm{i}\theta_{ij}}(c_{i,\uparrow}^\dagger c_{j,\downarrow}^\dagger - c_{i,\downarrow}^\dagger c_{j,\uparrow}^\dagger)+\mathrm{h.c.})$$



Charge-U(1) symmetry:

$$c_{i,\sigma} \rightarrow c_{i,\sigma}e^{\mathrm{i}\varphi}, \;\; \theta \rightarrow \theta + 2\varphi$$

$e^{i\theta}$ ~ fluctuating cooper pair

[Xiao Yan Xu, TG 2020]

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Charge-U(1) symmetry:

$$c_{i,\sigma} \rightarrow c_{i,\sigma} e^{\mathrm{i}\varphi}, \ \theta \rightarrow \theta + 2\varphi$$

$e^{i\theta}$ ~ fluctuating cooper pair

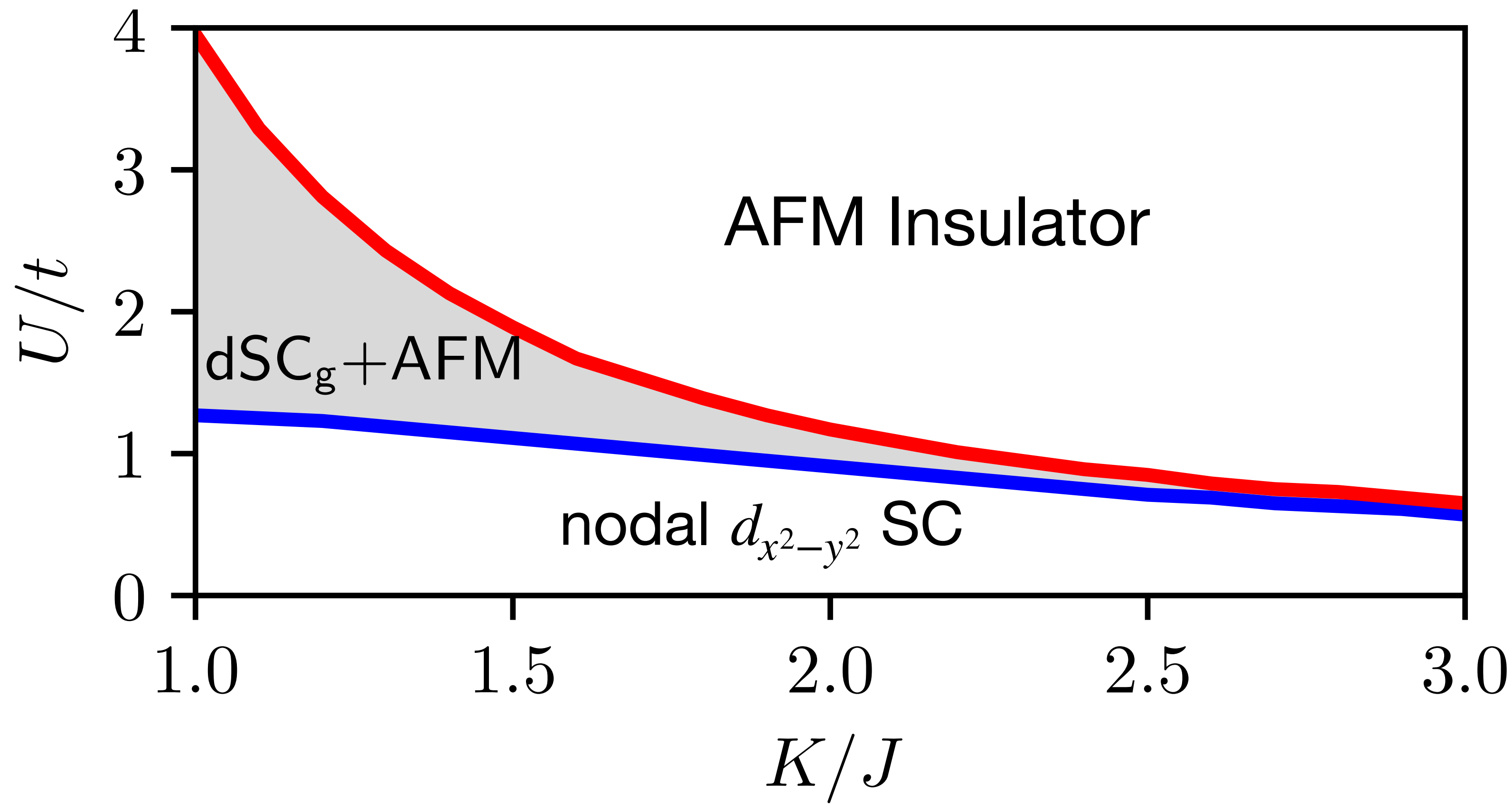
<u>Limits:</u>

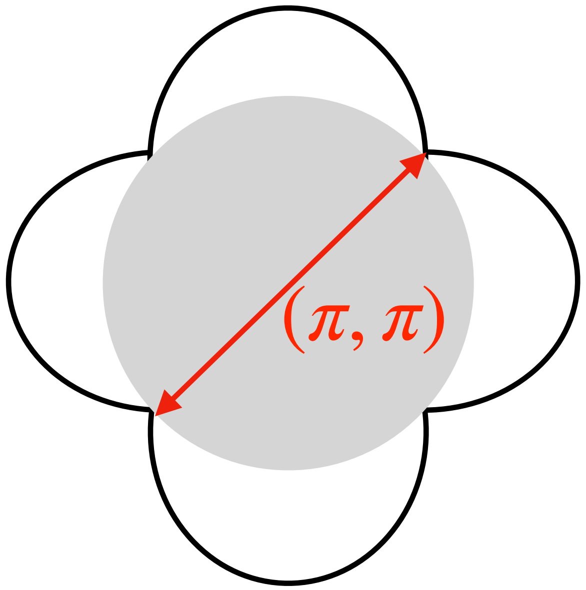
U, t >> J, K : AFM insulator

J, t >> K, U: nodal d-wave

[Xiao Yan Xu, TG 2020]

Mean-Field Phase Diagram





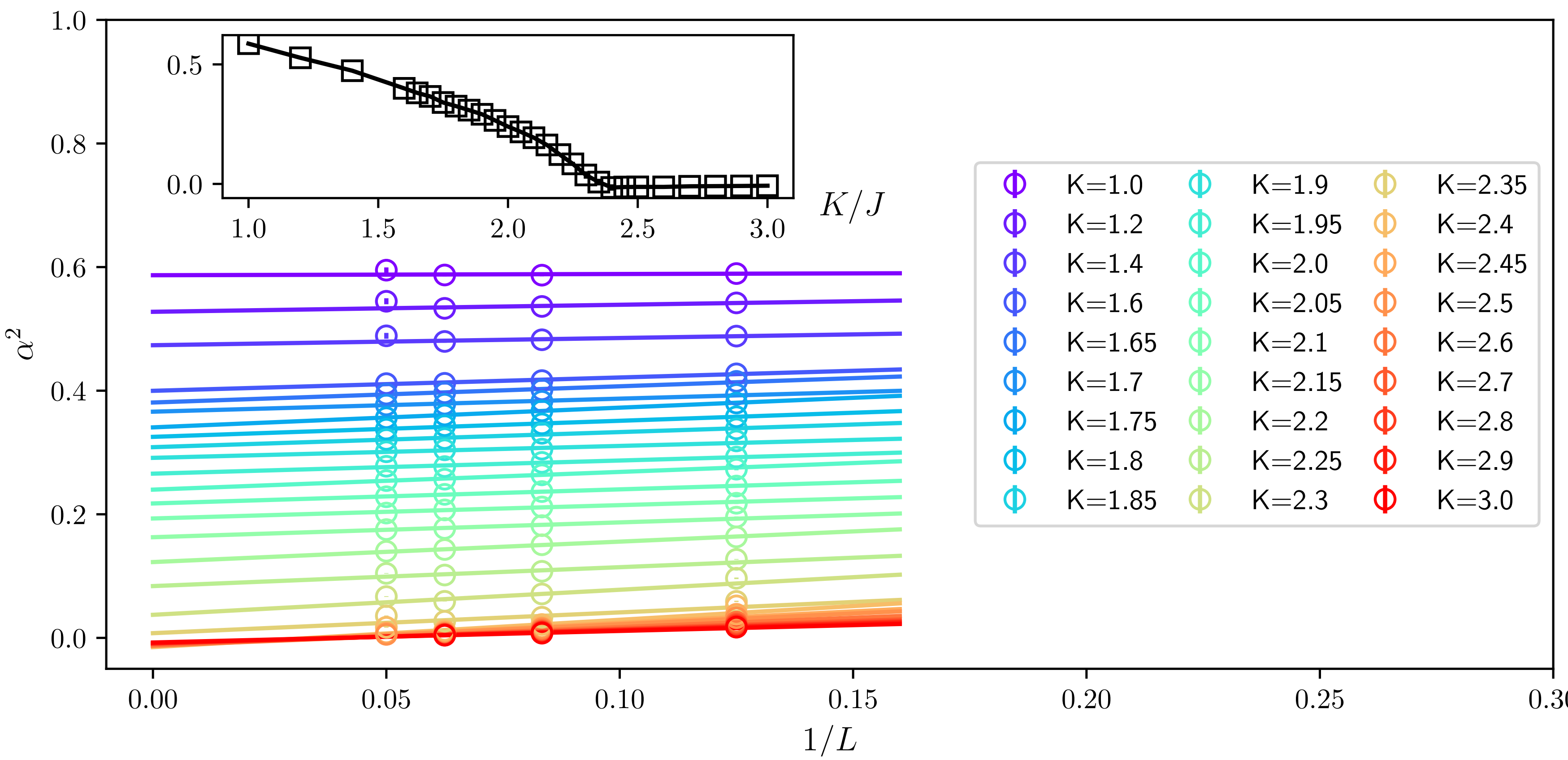
$$H = H_t + H_U + H_V + H_{XY}$$

$$H_{\mathrm{XY}} = K \sum_{\langle ij \rangle} n_{ij}^2 - J \sum_{\langle ij, il \rangle} \cos(\theta_{ij} - \theta_{il})$$

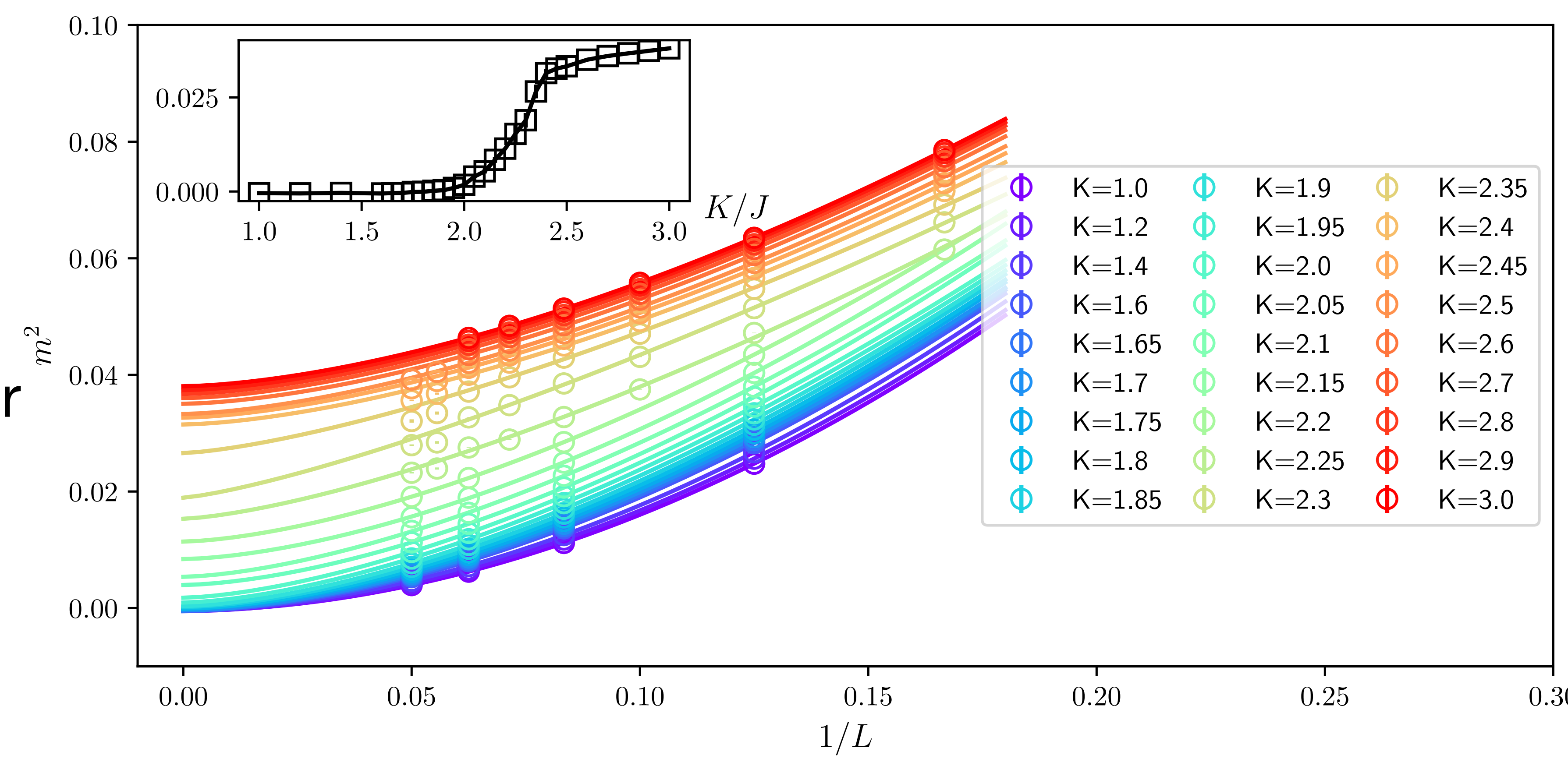
$$H_V = V \sum_{\langle ij \rangle} (\tau_{i,j} e^{\mathrm{i}\theta_{ij}} (c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} - c^\dagger_{i,\downarrow} c^\dagger_{j,\uparrow}) + \mathrm{h.c.})$$

Quantum Monte Carlo Results: Order Parameters

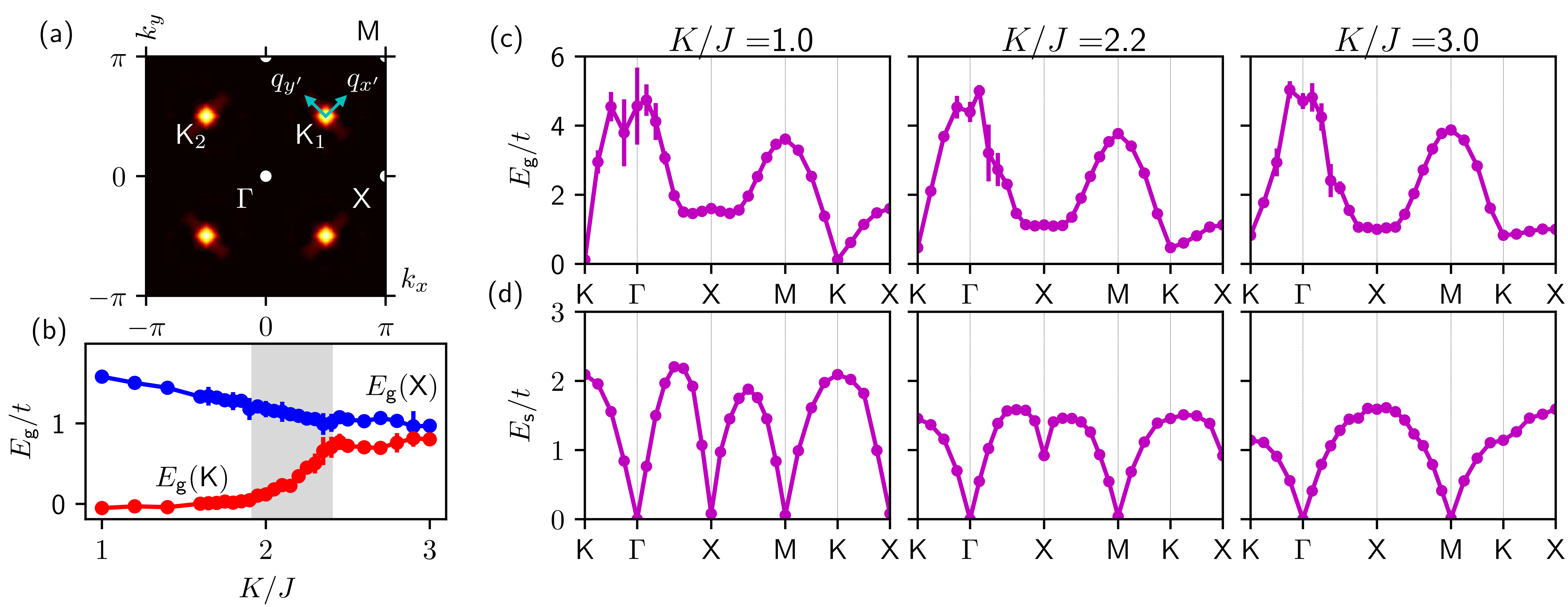
d-wave order parameter



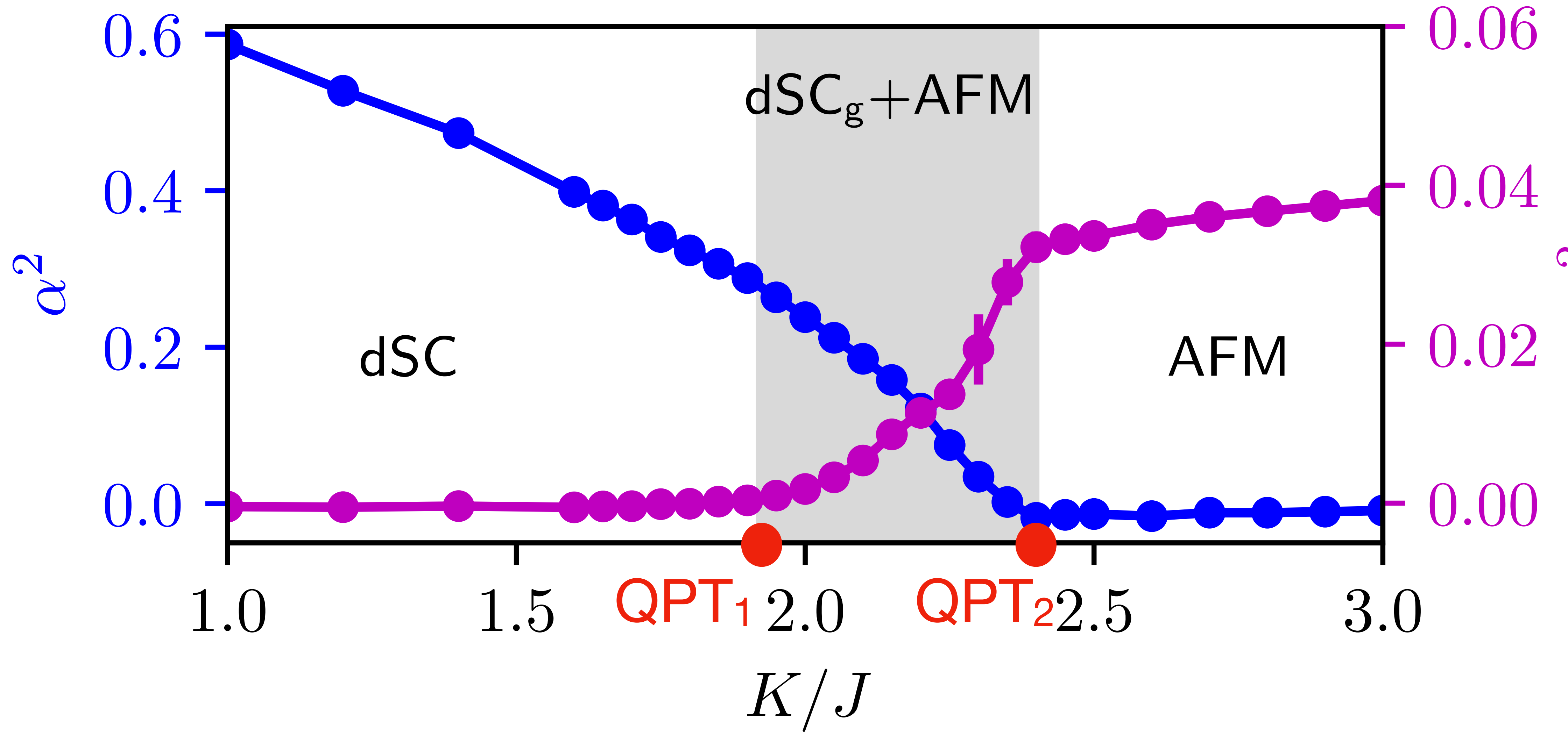
AFM order parameter



Quantum Monte Carlo Results: Spectral function and gaps

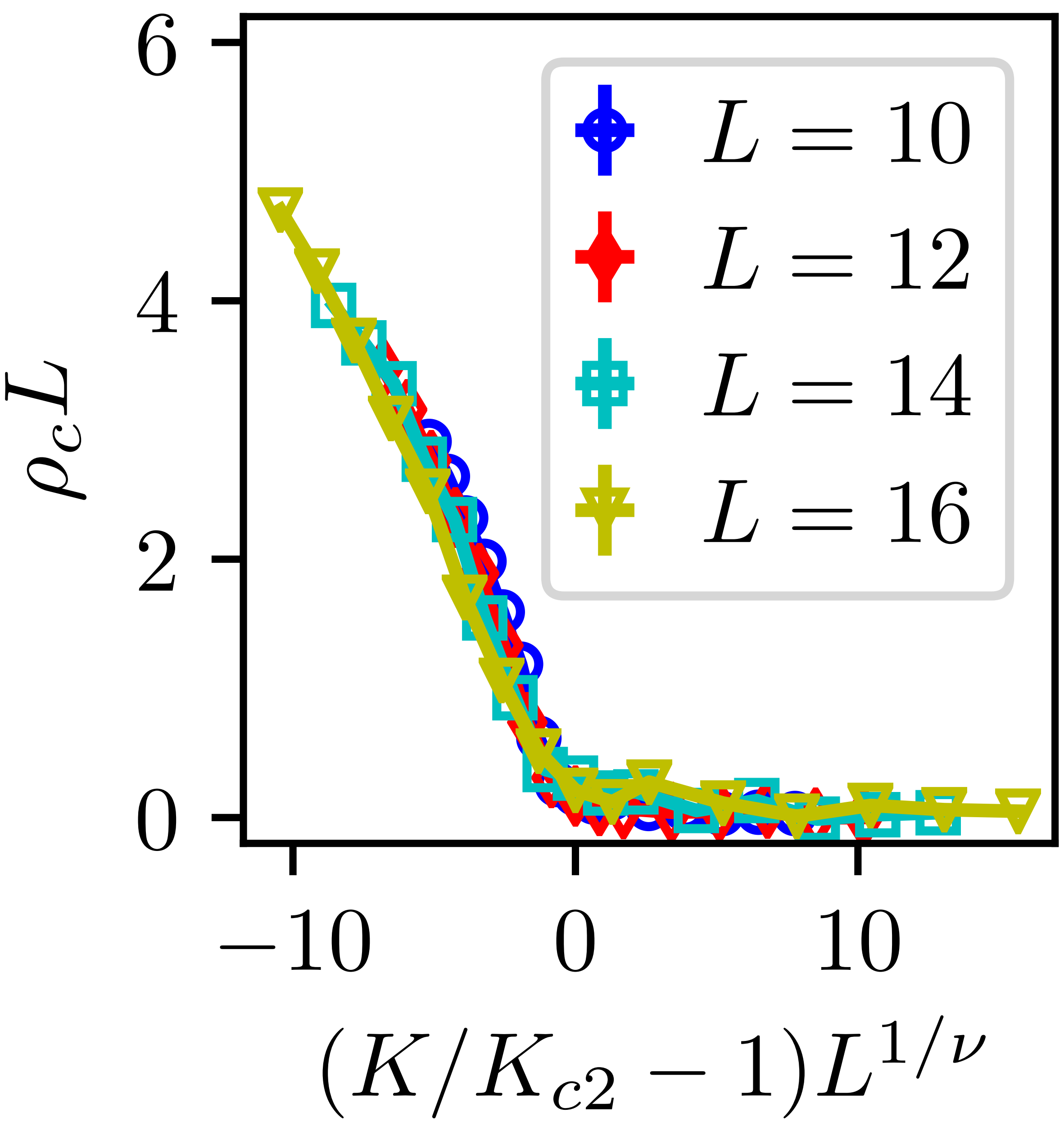


Nature of Quantum Phase Transitions?

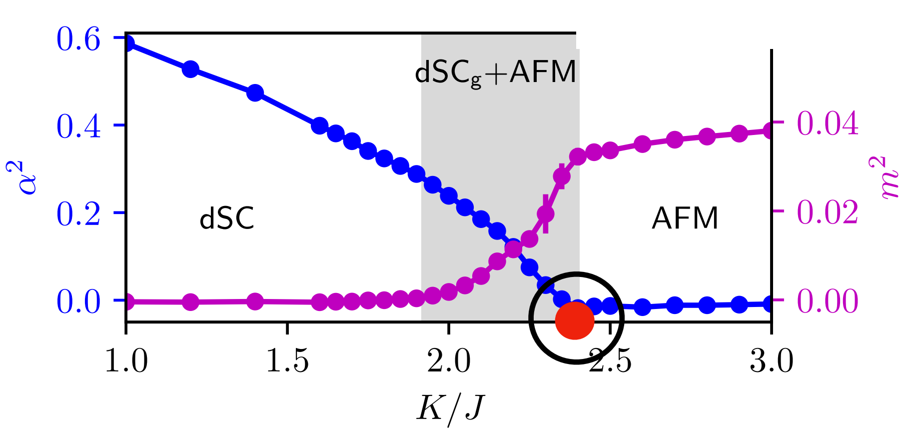


Transition from dSC to co-existence phase

ρ_c = superfluid stiffness.

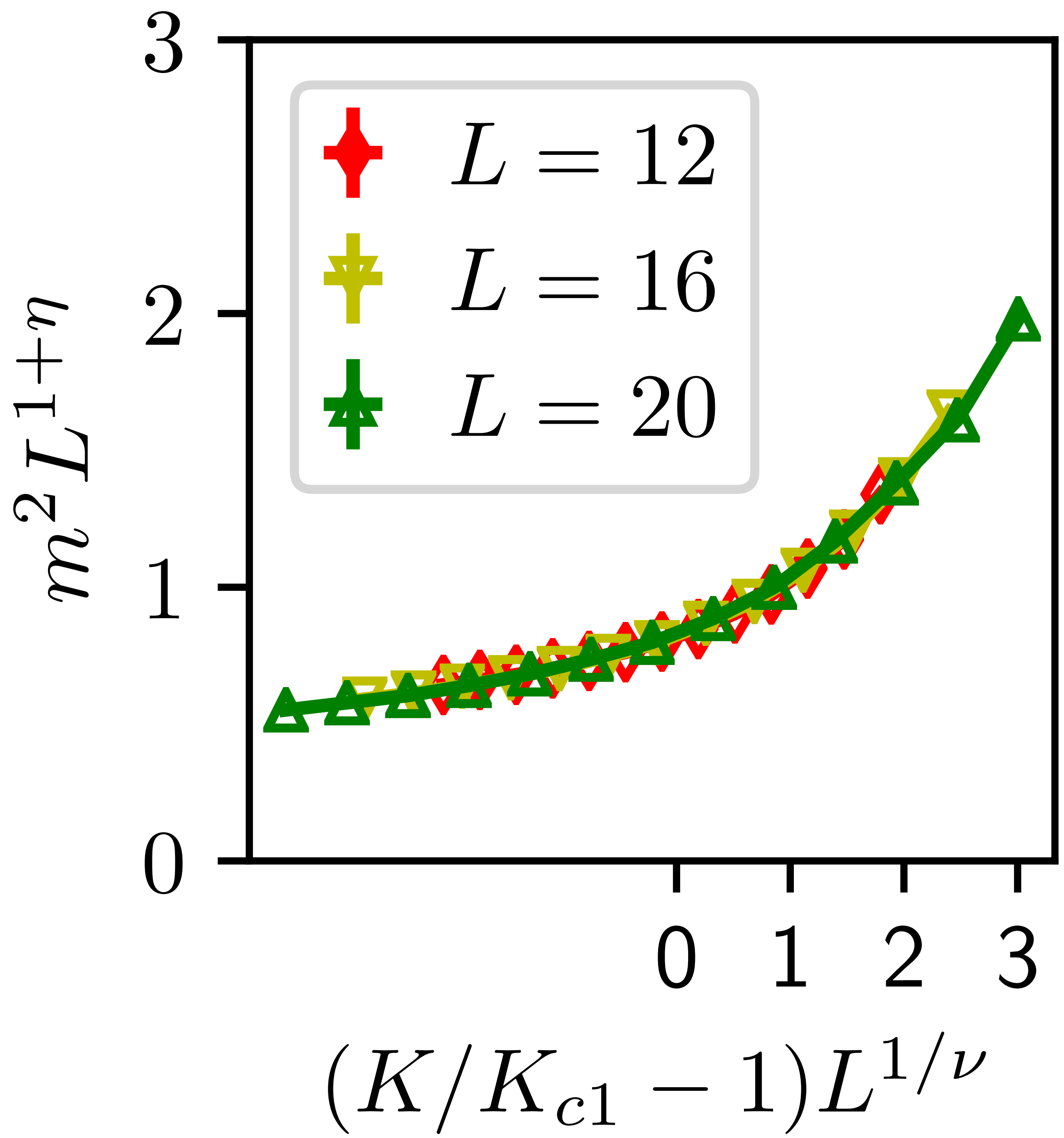


Exponents match 3D XY universality, as expected.



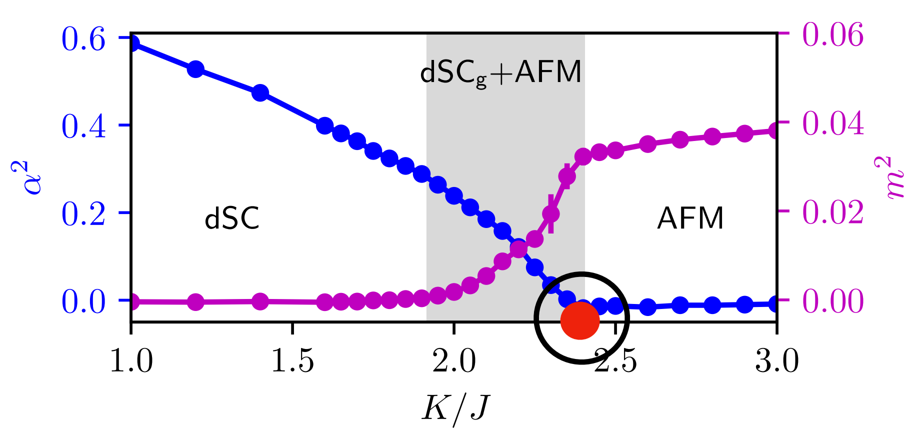
Transition from AFM to co-existence phase

m = AFM order parameter.

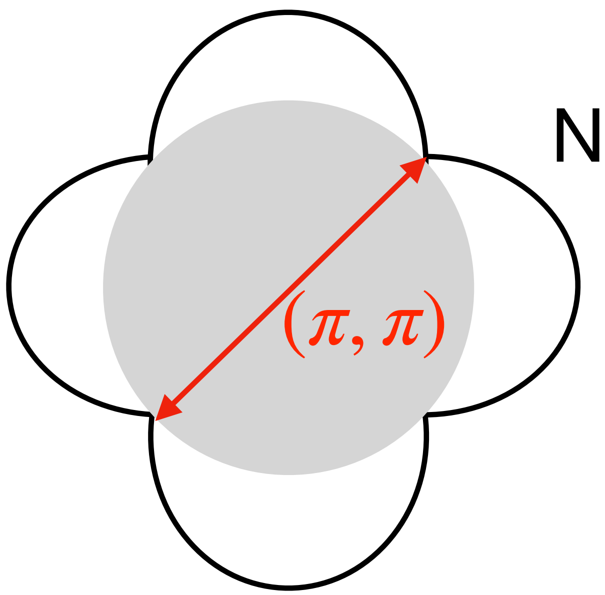


Scaling collapse yields

$\nu \approx 1, \eta_m \approx 0.55$



Field theory for dSC to co-existence transition

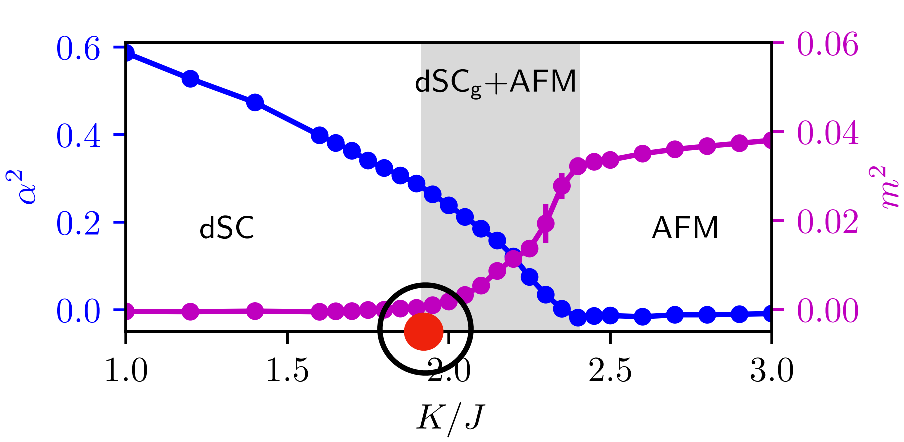


Nodal dirac fermions gapped out by Neel order parameter.

NODAL LIQUID THEORY OF THE PSEUDO-GAP PHASE OF HIGH-T_c SUPERCONDUCTORS

LEON BALENTS, MATTHEW P. A. FISHER and CHETAN NAYAK
Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106-4030, USA

(1998)



Field theory for dSC to co-existence transition

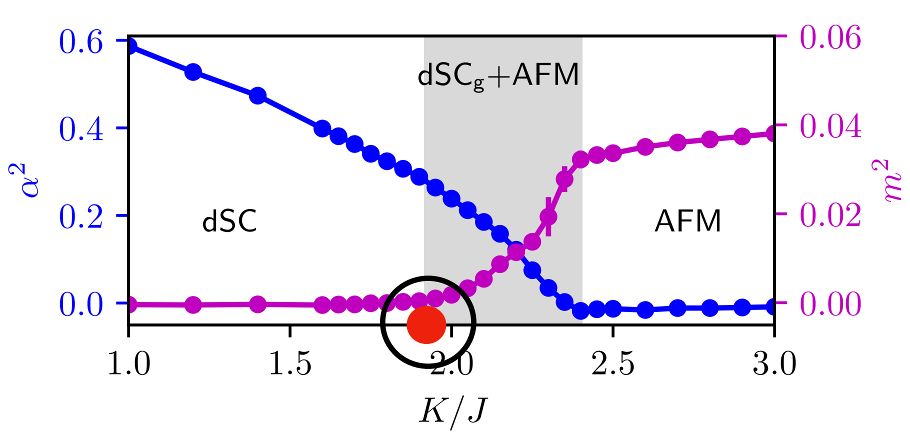
$$\mathcal{L} = \bar{\Psi}\partial\!\!\!/\Psi + \frac{1}{2}(\partial_\mu \vec{N})^2 + u(\vec{N}^2)^2 + g\vec{N}\cdot(\Psi^\dagger \tau^y \vec{\sigma}\sigma^y \Psi^\dagger + \text{h.c.})$$

[Balents, Fisher, Nayak 1998]

Ψ = eight component fermion (two Dirac spinor, two spin and two valley indices).

$\overrightarrow{N}$ = Neel order parameter field.

Critical theory breaks charge-U(1) since this symmetry is broken spontaneously on either sides of the transition.



We have set all three velocities v_F (Fermi velocity), v_Δ (nodal velocity), v_s (spin-wave velocity) equal to each other, as implied by the RG flow.

Mapping the field theory to more well-known form

Consider the unitary transformation:

$$\Psi'_\uparrow = \frac{1}{\sqrt{2}}\left(\Psi_\uparrow - i\,\Psi^\dagger_\downarrow\right) \qquad \Psi'_\downarrow = \frac{1}{\sqrt{2}}\left(\Psi_\downarrow + i\,\Psi^\dagger_\uparrow\right)$$

In new variables, one obtains standard Chiral Gross-Neveu-Heisenberg:

$$\mathcal{L} = \bar{\Psi}'\partial\!\!\!/\Psi' + \frac{1}{2}(\partial_\mu \vec{N})^2 + u(\vec{N}^2)^2 + 2g\vec{N}\cdot\bar{\Psi}'\vec{\sigma}\Psi'$$

Technically same as the theory for transition between neutral Graphene and AFM.

Well-studied using various techniques (ϵ-expansion, large-N, QMC, …)

Our exponents consistent with previous work.

Mapping the field theory to more well-known form

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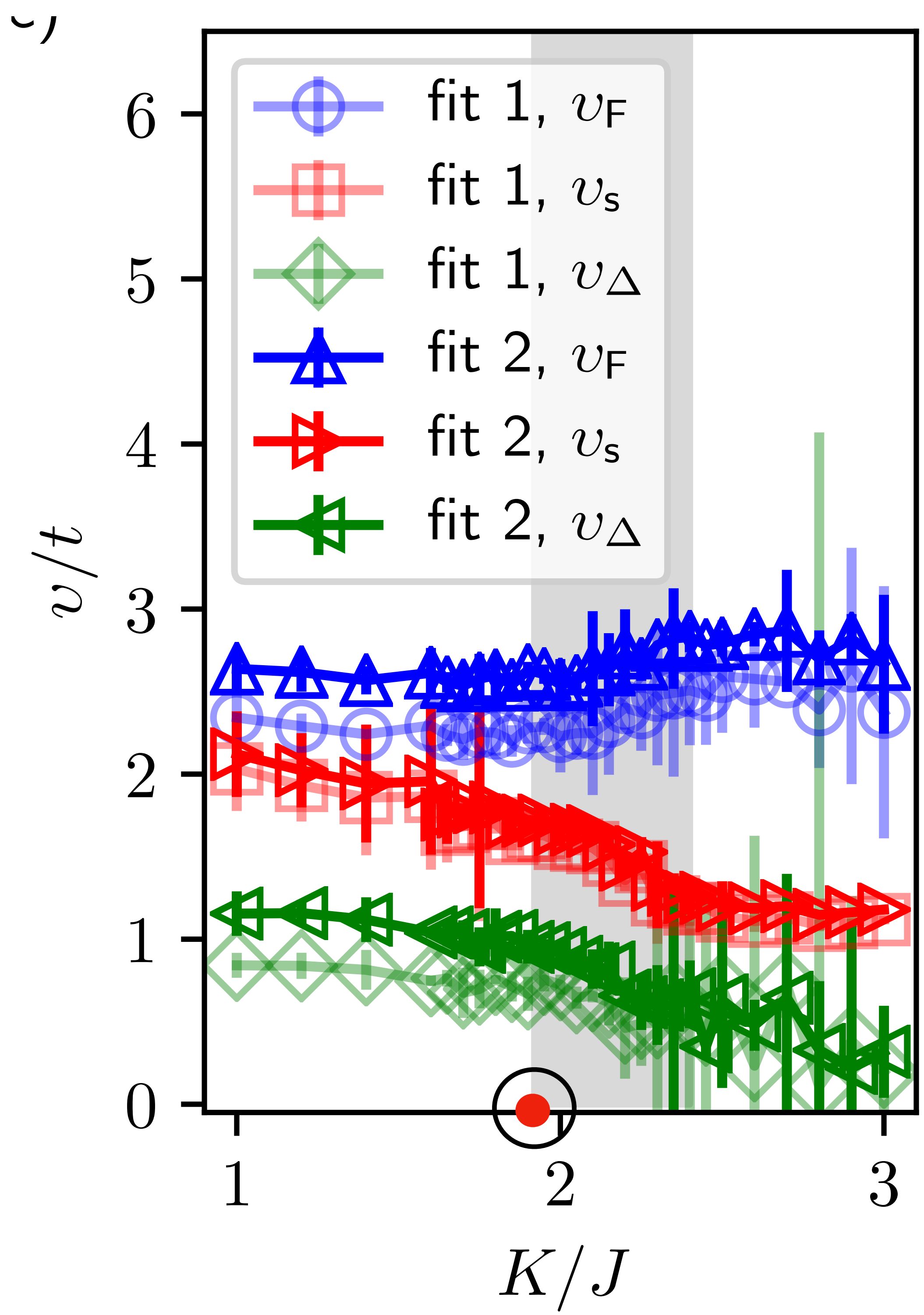
Related recent work by Otsuka et al: BCS mean-field for nodal d-wave + Hubbard U:

$$H = H_{\mathrm{BCS}} + H_U \qquad H_{\mathrm{BCS}} = \sum_{\langle i,j\rangle}\left\{\begin{pmatrix} c^\dagger_{i\uparrow} & c_{i\downarrow}\end{pmatrix}\begin{pmatrix} -t & \Delta_{ij} \\ \Delta^*_{ij} & t\end{pmatrix}\begin{pmatrix} c_{j\uparrow} \\ c^\dagger_{j\downarrow}\end{pmatrix} + \mathrm{h.c}\right\}$$

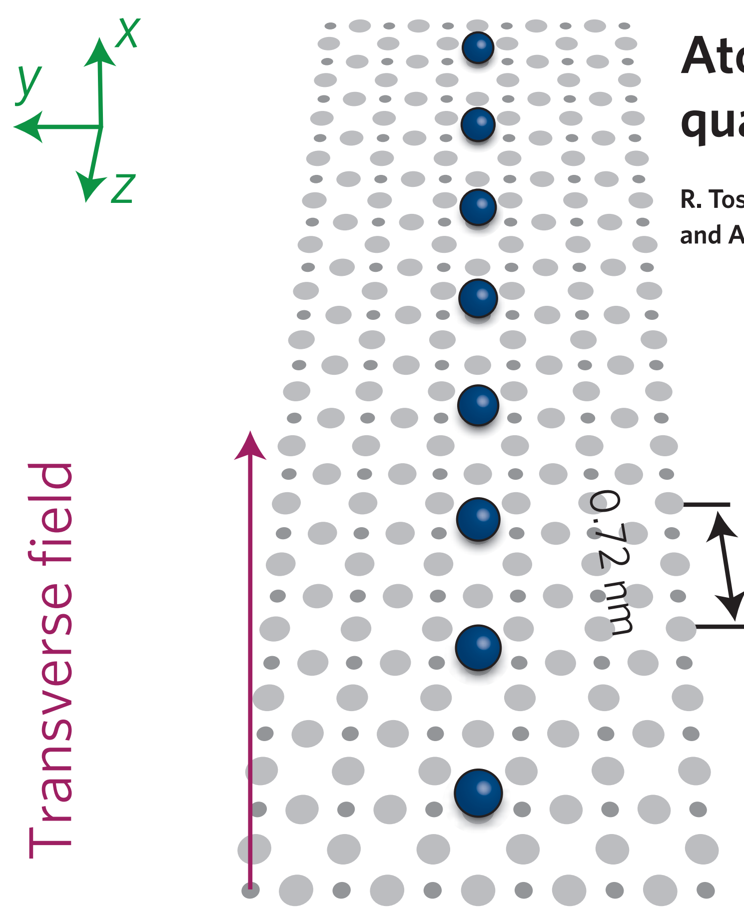
Velocity Renormalization?



Some tendency visible for velocities to become equal at transition.

The RG flow is logarithmically slow, so most likely need very large sizes to see equality of velocities.

Part-II: Motivation

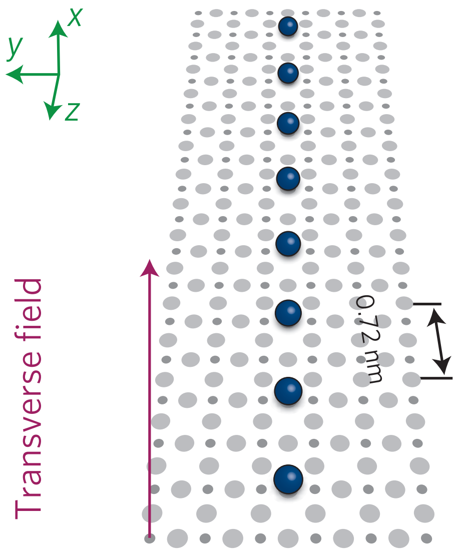


Atomic spin-chain realization of a model for quantum criticality (2016)

R. Toskovic[1†], R. van den Berg[2†], A. Spinelli[1], I. S. Eliens[2], B. van den Toorn[1], B. Bryant[1], J.-S. Caux[2] and A. F. Otte[1*]

Magnetic cobalt adatoms on metallic copper.

Part-II: Motivation



[Toskovic et al (2016)]

Coupling with Cu substrate leads to an effective Kondo lattice model.

[Danu, Assaad, Mila (2019)]

$$\hat{H} = -t\sum_{\langle i,j\rangle,\sigma}(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \mathrm{H.c.}) + J_k\sum_{l=1}^{L}\hat{\mathbf{S}}^{c}_{l}\cdot\hat{\mathbf{S}}_{l}$$

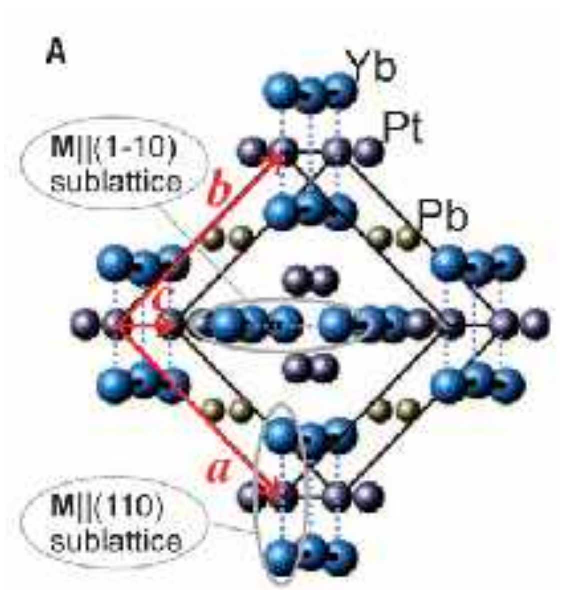
$$+ J_h\sum_{l=1}^{L-1}\hat{\mathbf{S}}_{l}\cdot\hat{\mathbf{S}}_{l+\Delta l} - g\mu_B h^z\sum_{l=1}^{L}\hat{S}^{z}_{l}.$$

Intermediate setting between a single-purity Kondo model, and conventional 2D Kondo lattice model.

Part-II: More motivation

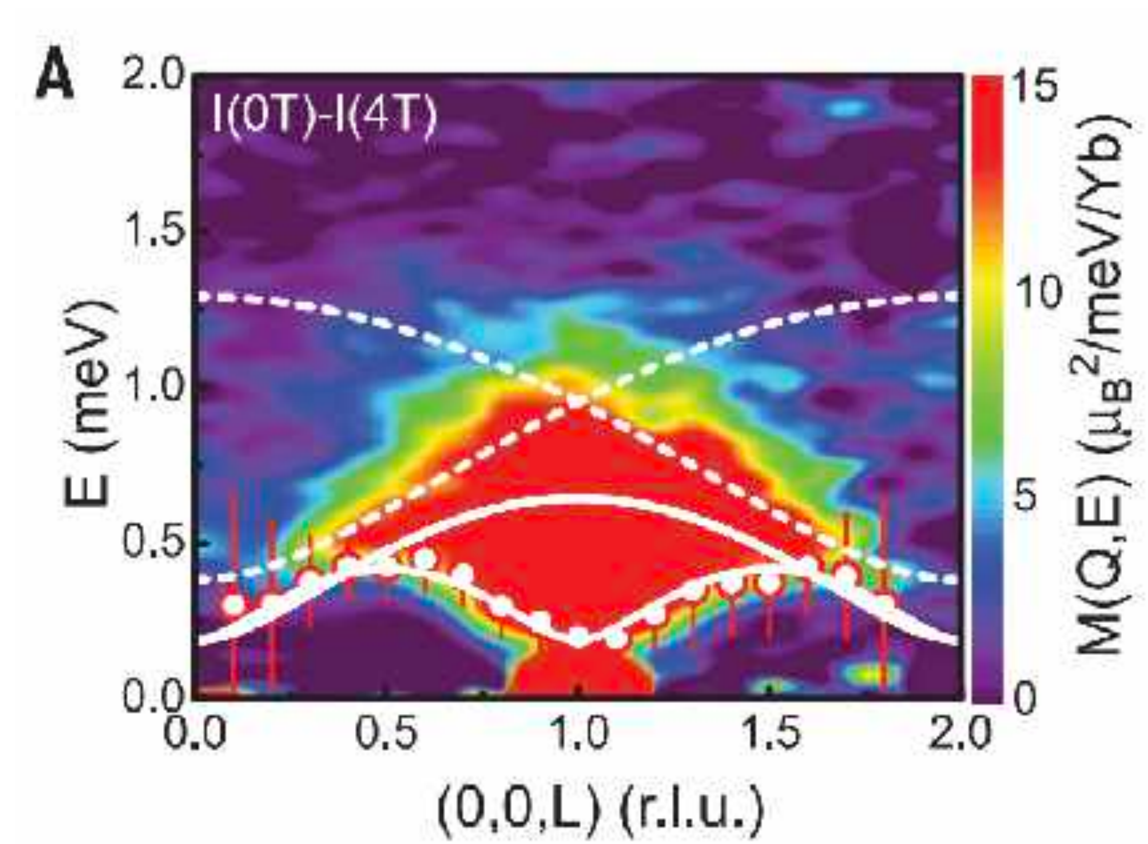
Orbital-exchange and fractional quantum number excitations in an f-electron metal, Yb_2Pt_2Pb

L. S. Wu,[1,2,3] W. J. Gannon,[1,2,4] I. A. Zaliznyak,[2*] A. M. Tsvelik,[2] M. Brockmann,[5,6] J.-S. Caux,[6] M. S. Kim,[2] Y. Qiu,[7] J. R. D. Copley,[7] G. Ehlers,[3] A. Podlesnyak,[3] M. C. Aronson[1,2,4]



[Wu et al 2016; Classen et al 2018; Gannon et al 2019]

Evidence of spin-1/2 spinons despite good 3D metal. Apparent "Kondo breakdown".



"De-signer" models

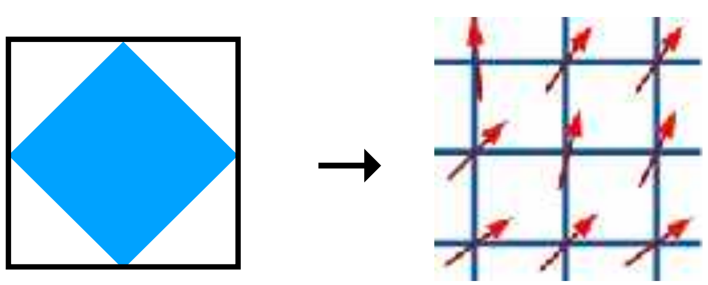
Pick your poison…

Want Mott Physics… Vs Want Fermi surfaces …

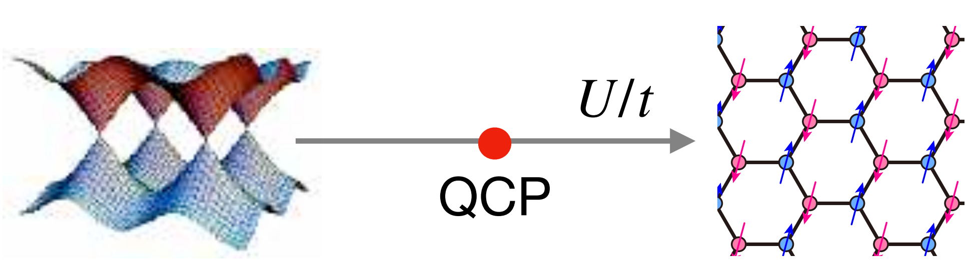
Main caveat:

Restricted to half-filling and bipartite lattices.

- Fermi surface nesting, leading to immediate AFM instability.



- Dirac semi-metal competing with AFM.



[Assaad, Herbut 2013; Otsuka et al 2016,…]

Typically (not always), multi-band Hubbard models with inter-band repulsion and intra-band onsite attraction.

[Wu, Zhang 2005]

Can capture some competing orders such as nematic, spin-density wave, non-nodal SC.

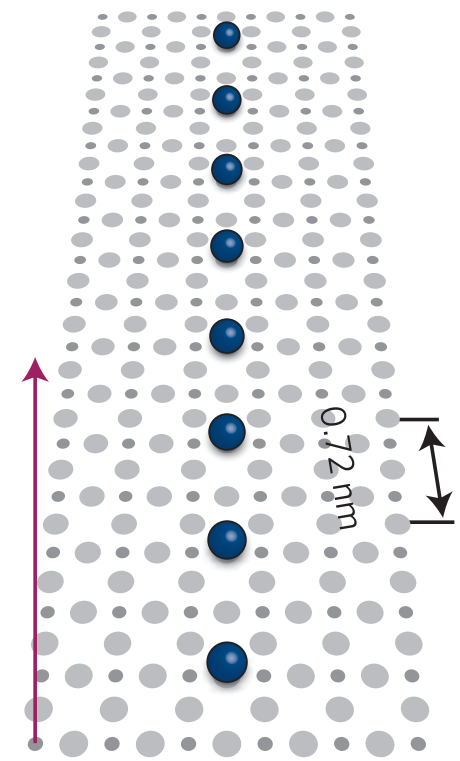
[Berg et al 2012; Schattner et al 2015; Dumitrescu et al 2016; Li et al 2017; Lederer et al 2017; Wang et al 2017, …]

Main caveat: no Mott physics, no nodal SC, s-wave SC can lurk at low-T which can obscure T = 0 QCP.

A model for Kondo breakdown in metal

1d spin-chain on a Dirac semi-metal.

$$\hat{H} = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle,\sigma} \left(e^{\frac{2\pi i}{\Phi_0}\int_i^j \boldsymbol{A}.\boldsymbol{dl}}\, \hat{\boldsymbol{c}}_{\boldsymbol{i}}^{\dagger}\hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c. \right) + \frac{J_k}{2}\sum_{\boldsymbol{l}=1}^{L} \hat{\boldsymbol{c}}_{\boldsymbol{l}}^{\dagger}\boldsymbol{\sigma}\hat{\boldsymbol{c}}_{\boldsymbol{l}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{l}} + J_h \sum_{\boldsymbol{l}=1}^{L} \hat{\boldsymbol{S}}_{\boldsymbol{l}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{l}+\Delta \boldsymbol{l}}$$

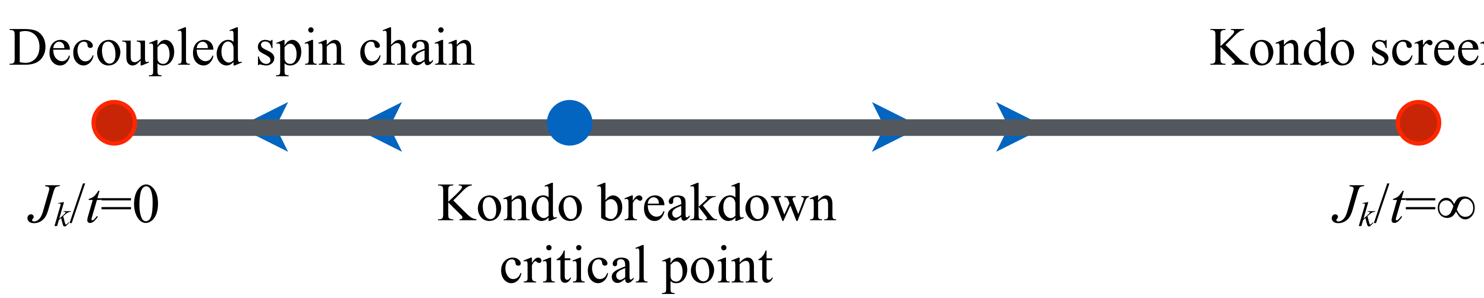


Low energy theory:

$$S = \int d^2x\, d\tau\ \bar{\Psi}\partial\!\!\!/\Psi + J_K \int dx\, d\tau\ \vec{N}\cdot\bar{\Psi}\vec{\sigma}\Psi + S_{\text{1d Heisenberg}}$$

Power-counting shows that J_K irrelevant at the decoupled fixed-point.

Guess:



[Danu, Vojta, Assaad, Grover (2020)]

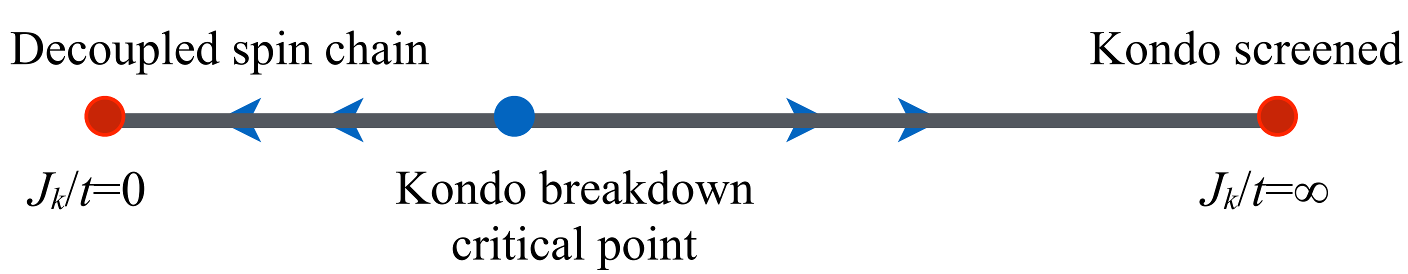
RG for Kondo breakdown transition

$$S = \int d^d x\, d\tau\ \bar{\Psi} \partial\!\!\!/ \Psi + J_K \int dx\, d\tau\ \vec{N} \cdot \bar{\Psi} \vec{\sigma} \Psi + S_{\text{1d Heisenberg}}$$

Kondo coupling marginal in d = 3/2 dimensions. Physical case: d = 2.

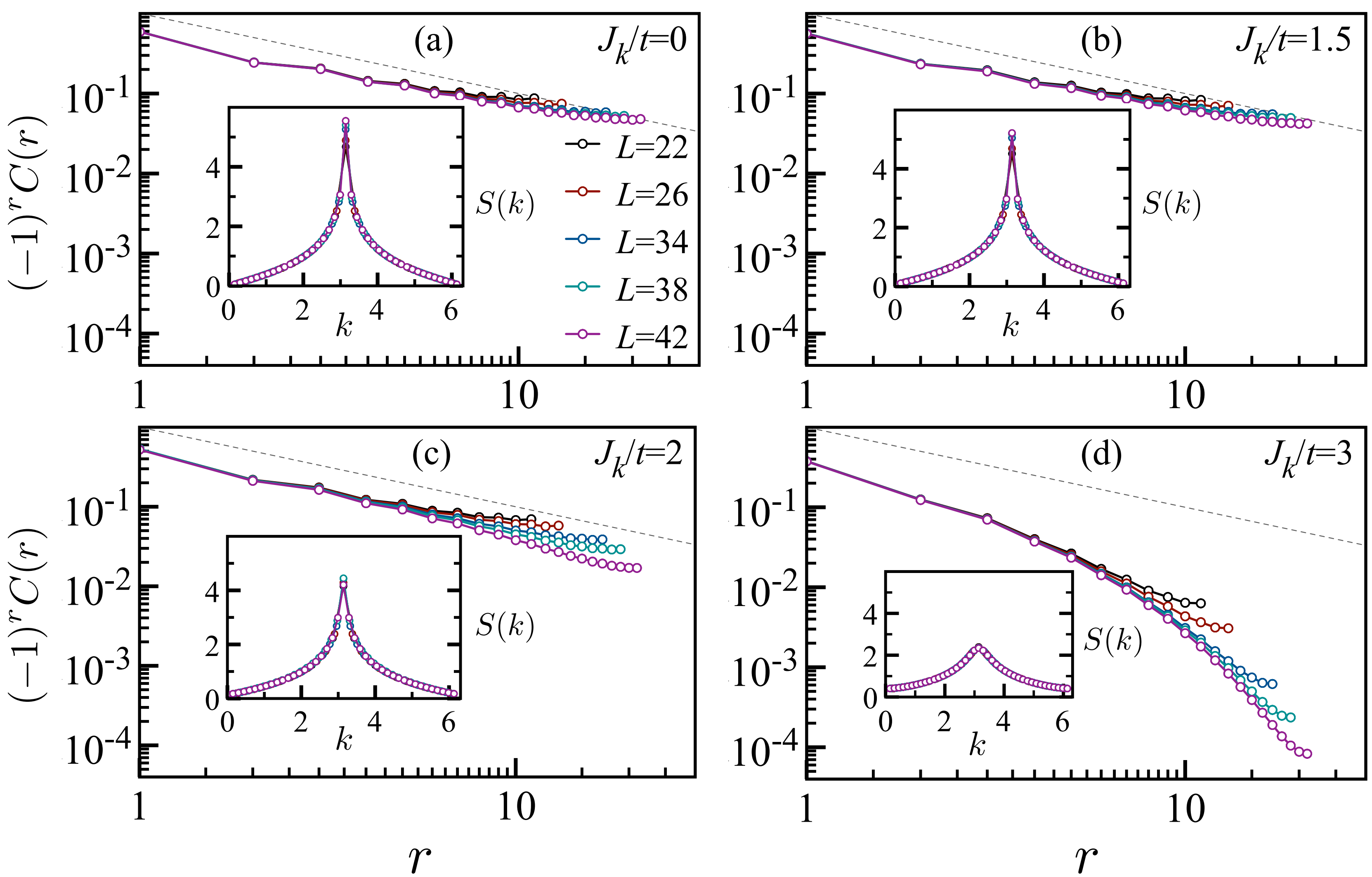
Perform RG using ε-expansion where ε = d-3/2, and finally set ε = 1/2.

$$\frac{dj_k}{d \ln \Lambda} = \epsilon j_k - \frac{j_k^2}{2} \qquad j_k = J_k \Lambda^{\epsilon}$$



Note: RG is being done by perturbing an *interacting* fixed-point, conformal perturbation theory useful.

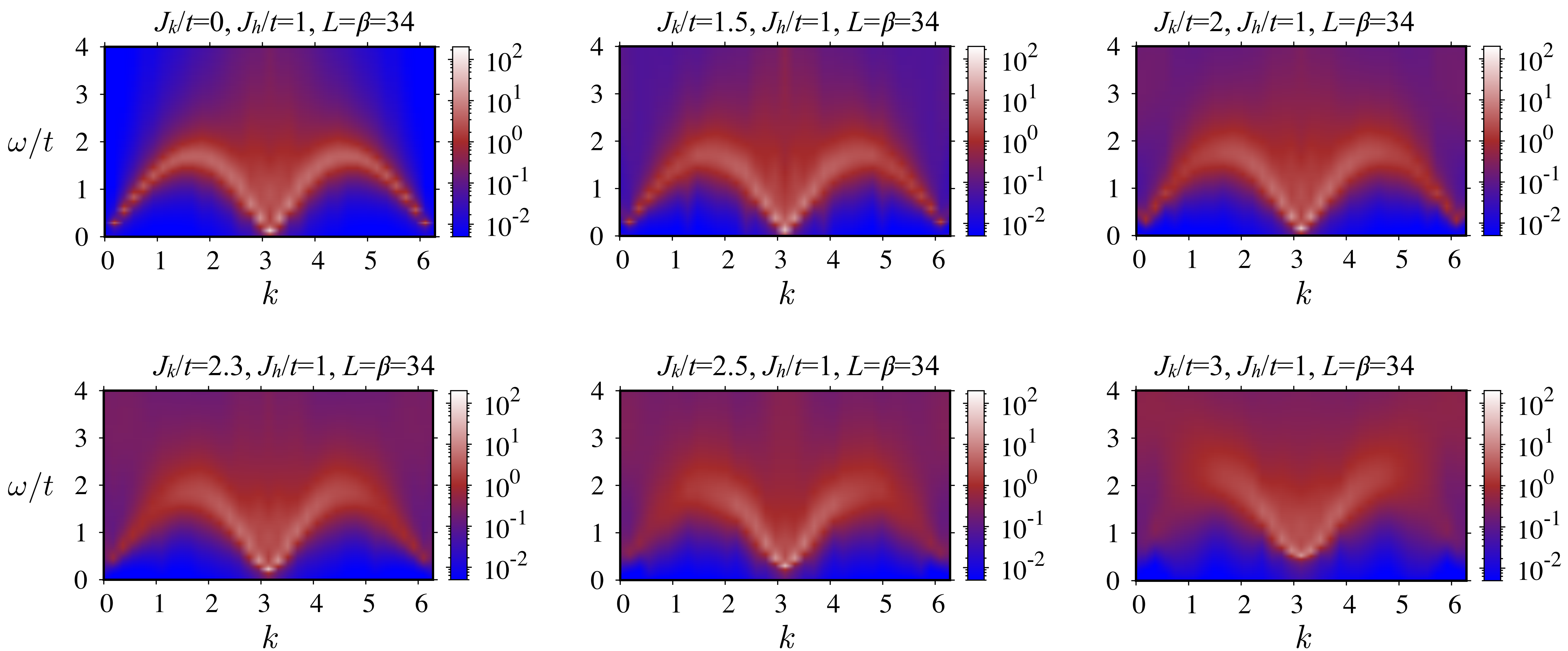
QMC simulations for Kondo breakdown



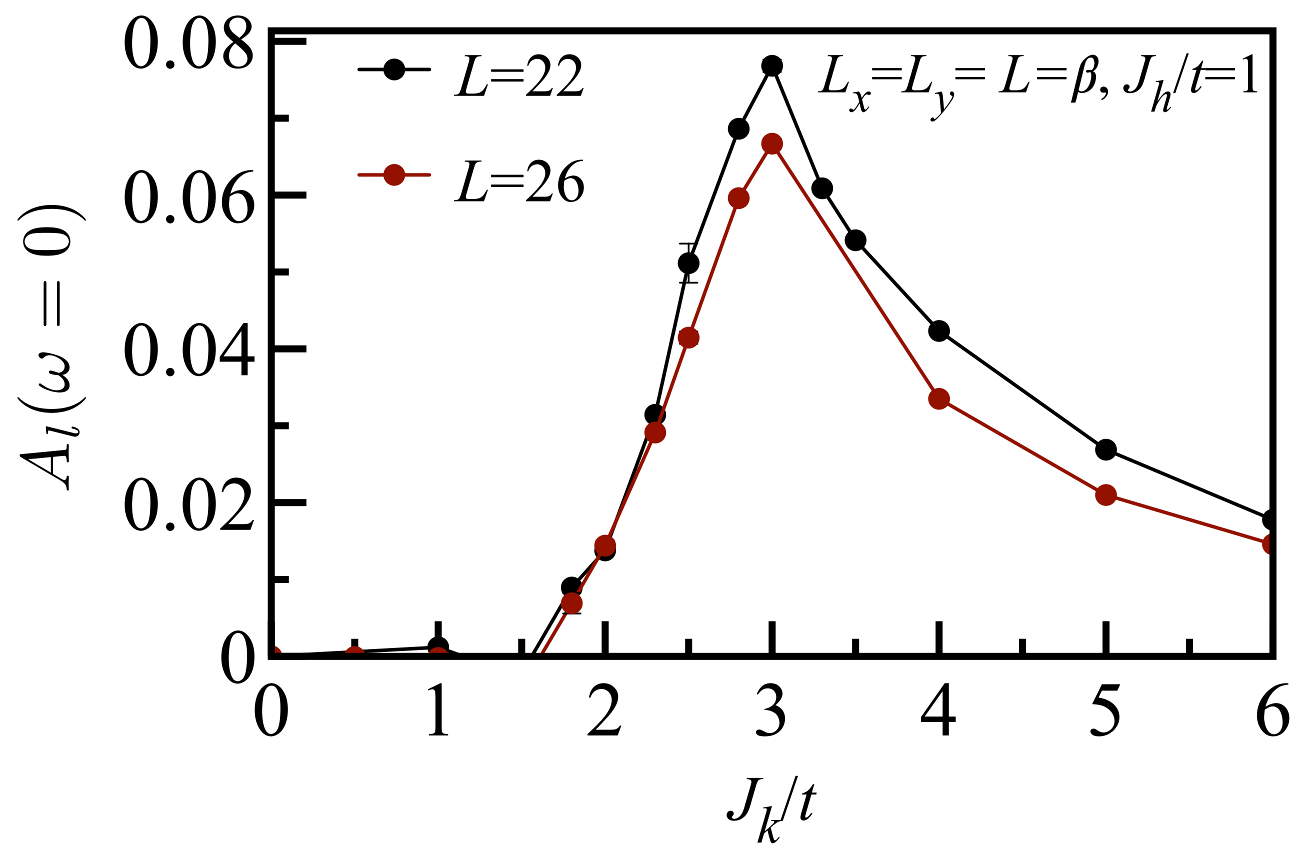
Spin-spin correlations decay as $(-1)^r\sqrt{\log(r)}/r$ for $J_K < J_{K,c}$

and as $(-1)^r/r^4$ for $J_K > J_{K,c}$

Spin-structure factor across Kondo breakdown transition



Zero-bias tunneling across Kondo breakdown transition



Kondo breakdown phase = fractionalized Fermi liquid

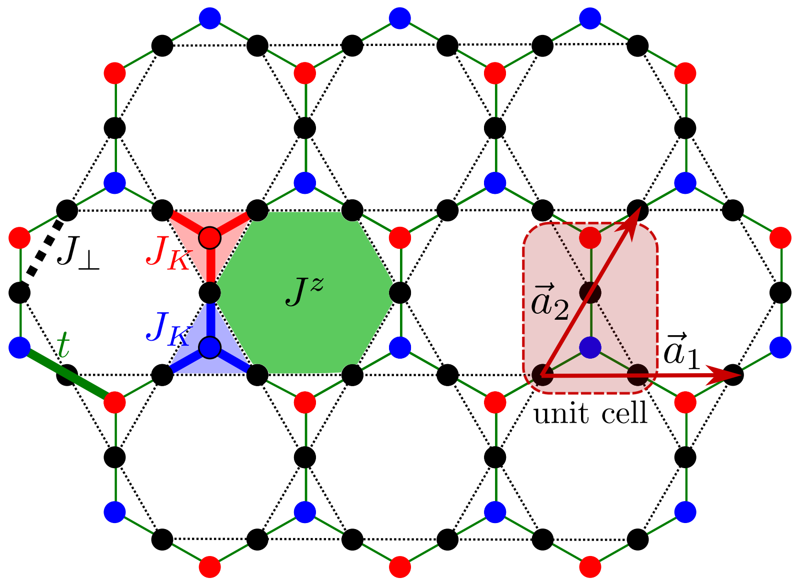
In the Kondo breakdown phase, the 1d spinons decouple from the 2d Dirac electrons. “Small Fermi surface phase”.

[Senthil, Vojta, Sachdev (2003)]

Here, the effect on bulk quantities rather “timid” due to dimensional mismatch. Only log(L) entanglement entropy missing due to breakdown.

Regular versions of fractionalized Fermi liquid?

A model for 2d Fractionalized Fermi liquid



● ● c fermions (honeycomb lattice)

● localized spins (kagome lattice)

$$\hat{H} = \hat{H}_c + \hat{H}_S + \hat{H}_K$$

$$\hat{H}_c = -t \sum_{\langle \boldsymbol{x},\boldsymbol{y}\rangle,\sigma} \hat{c}^\dagger_{\boldsymbol{x},\sigma}\hat{c}_{\boldsymbol{y},\sigma} + h.c.$$

$$\hat{H}_{\mathrm{S}} = -J^\perp \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle} \left(\hat{S}^{f,+}_{\boldsymbol{i}}\hat{S}^{f,-}_{\boldsymbol{j}} + h.c.\right) + J^z \sum_{\hexagon} \left(\hat{S}^{f,z}_{\hexagon}\right)^2$$

$$\hat{H}_K = J_K \sum_{\langle \boldsymbol{x},\boldsymbol{i}\rangle} \left[\hat{S}^{c,z}_{\boldsymbol{x}}\hat{S}^{f,z}_{\boldsymbol{i}} - (-1)^{\boldsymbol{x}}\left(\hat{S}^{c,+}_{\boldsymbol{x}}\hat{S}^{f,-}_{\boldsymbol{i}} + h.c.\right)\right]$$

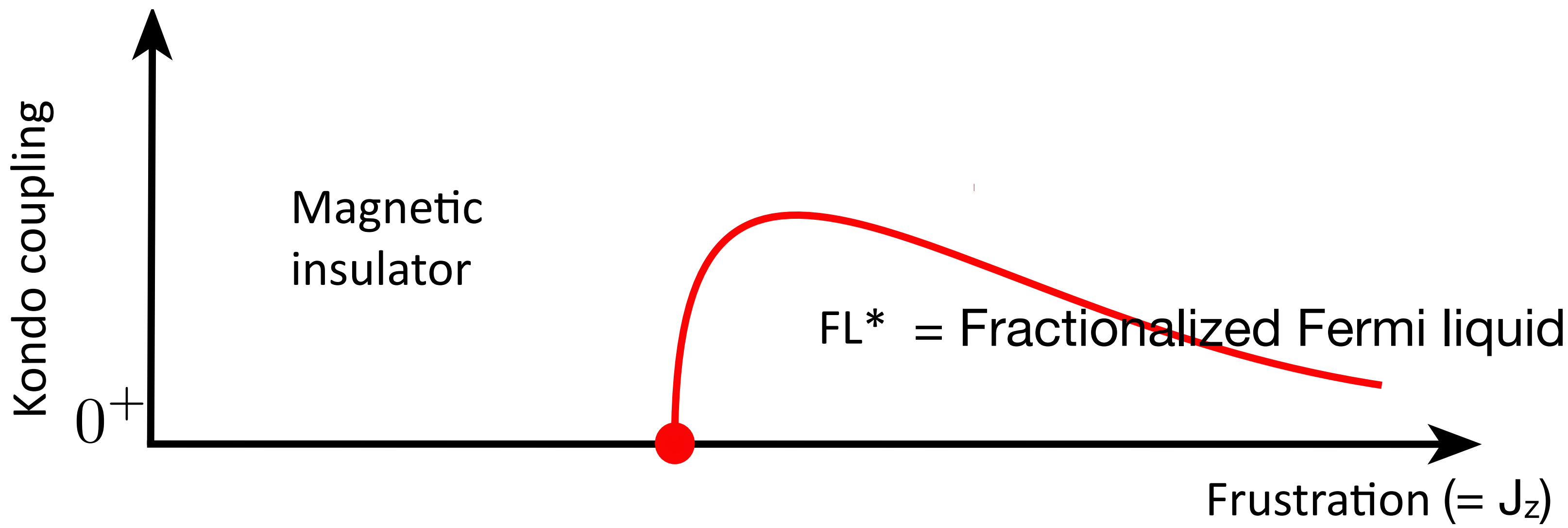
[Hofmann, Assaad, TG 2018]

H_s is the Balents-Fisher-Girvin model that supports a topologically ordered Z_2 spin-liquid when $J^z >> J^\perp$

Surprisingly, the above model does not have a sign-problem, by employing fermion representation of spins.

[Sato, Assaad, TG 2017]

Schematic Phase Diagram obtained from QMC

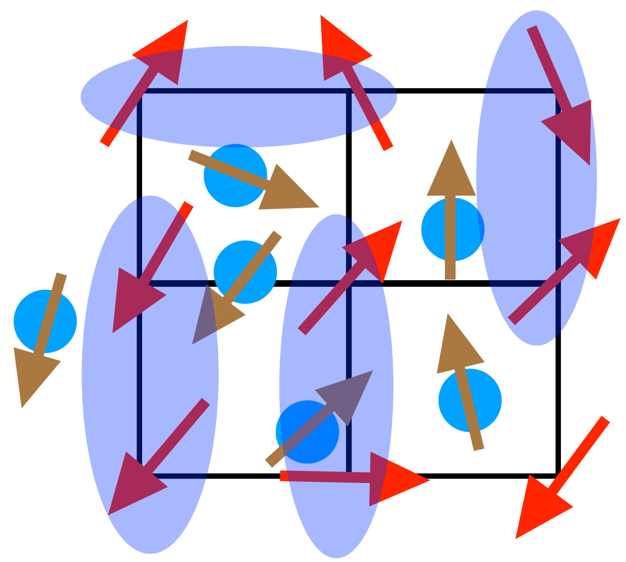


FL* phase has a small Fermi surface, i.e. violates Luttinger theorem, and has no non-trivial quadratic mean-field description.

The spins enter a Z_2 spin-liquid, and decouple from the conduction electrons which form a Dirac semi-metal.

[Hofmann, Assaad, TG 2018]

Cartoon of fractionalized Fermi liquid (FL*)



Spins form a gapped RVB state. The fermions decouple from spins and form a small Fermi surface.

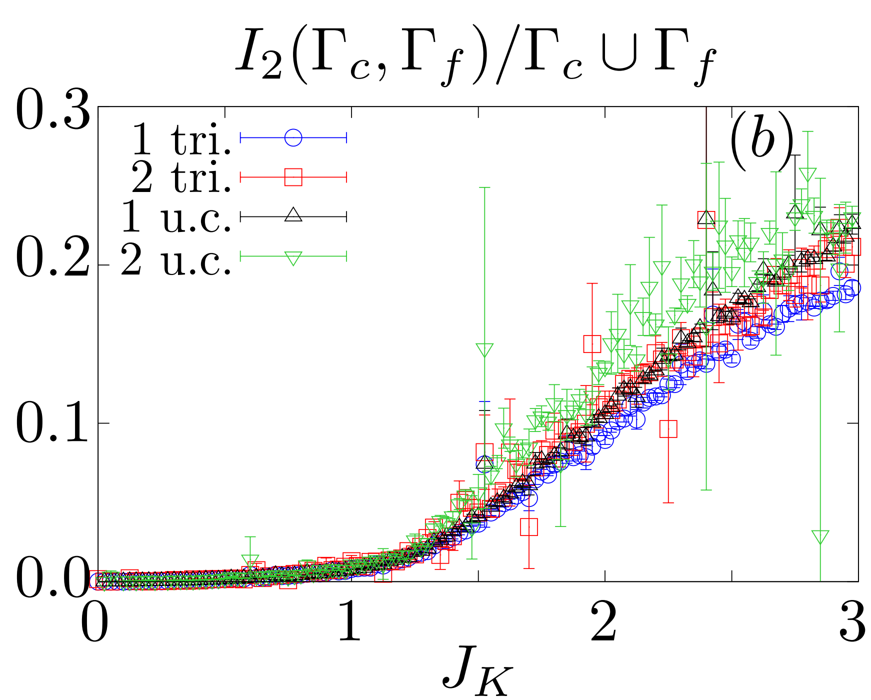
[Senthil, Vojta, Sachdev (2003)]

Characterizing Kondo Screening via Entanglement

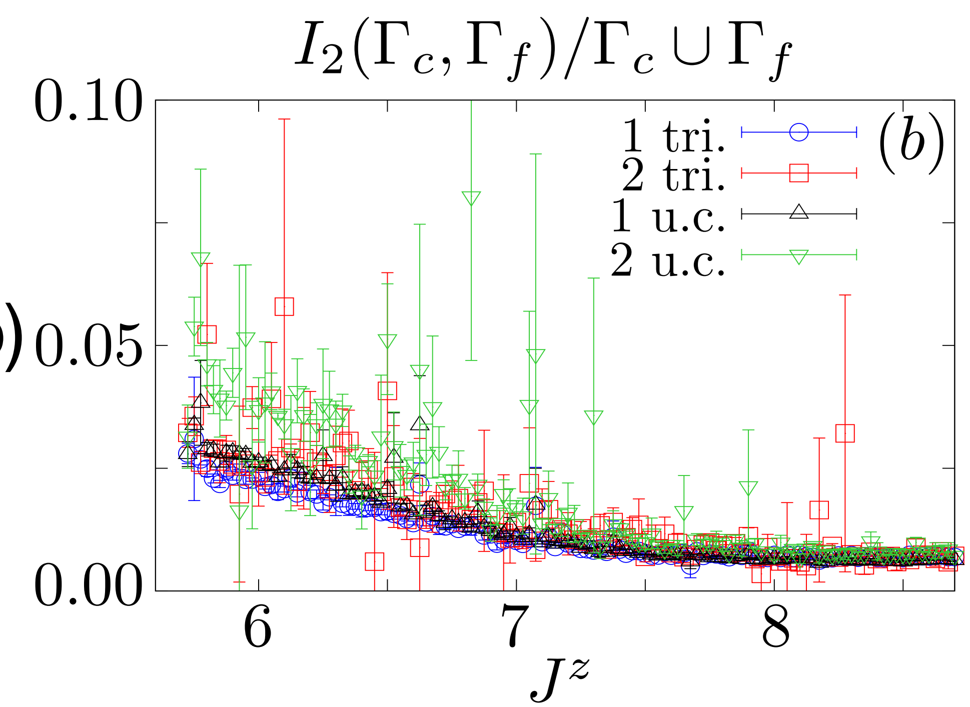
Renyi mutual information between conduction electrons and spins:

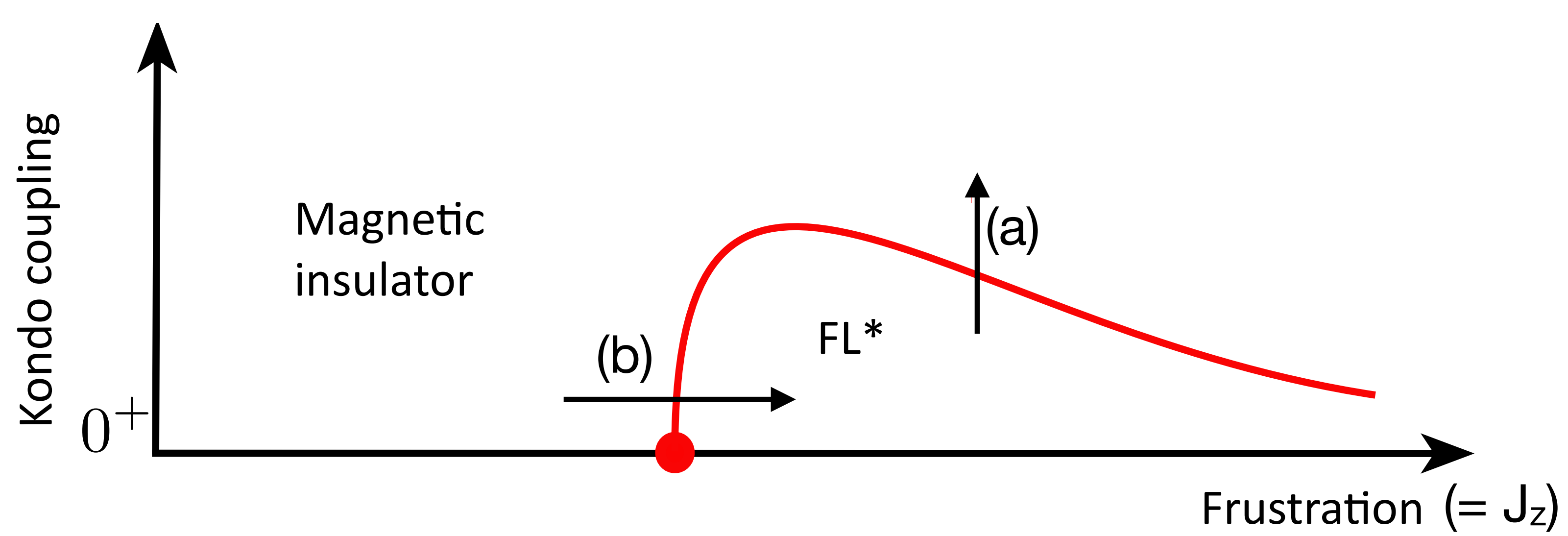
$$I_2(\Gamma_c, \Gamma_f) \equiv S_2(\Gamma_c \cup \Gamma_f) - S_2(\Gamma_c) - S_2(\Gamma_f)$$

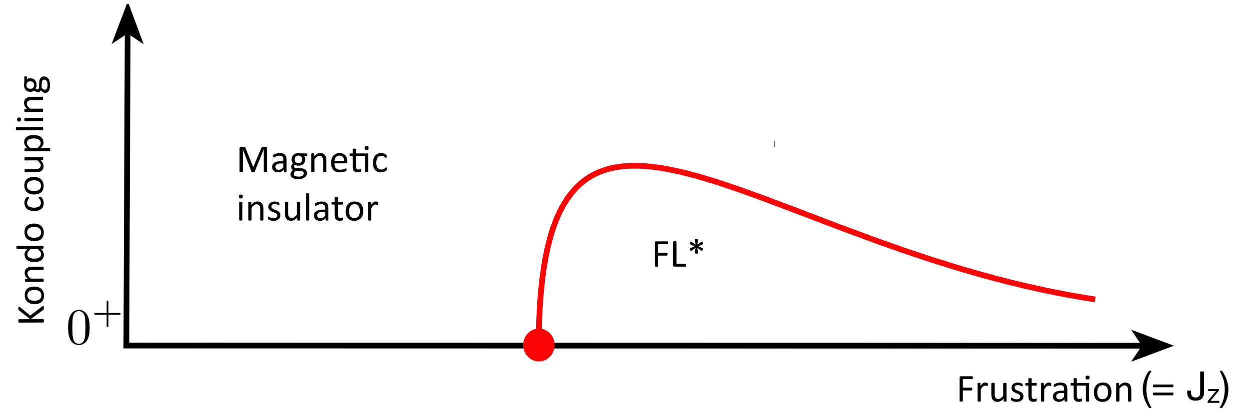
(a)



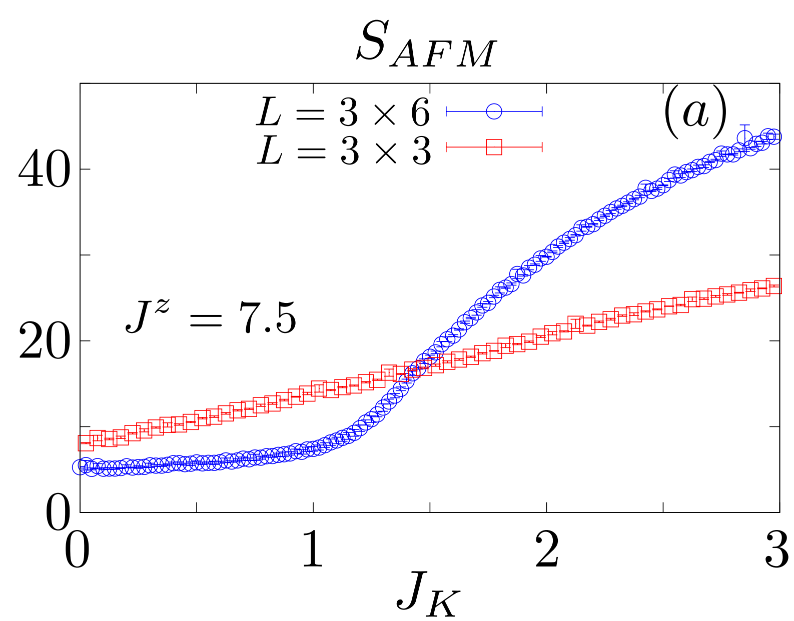
(b)

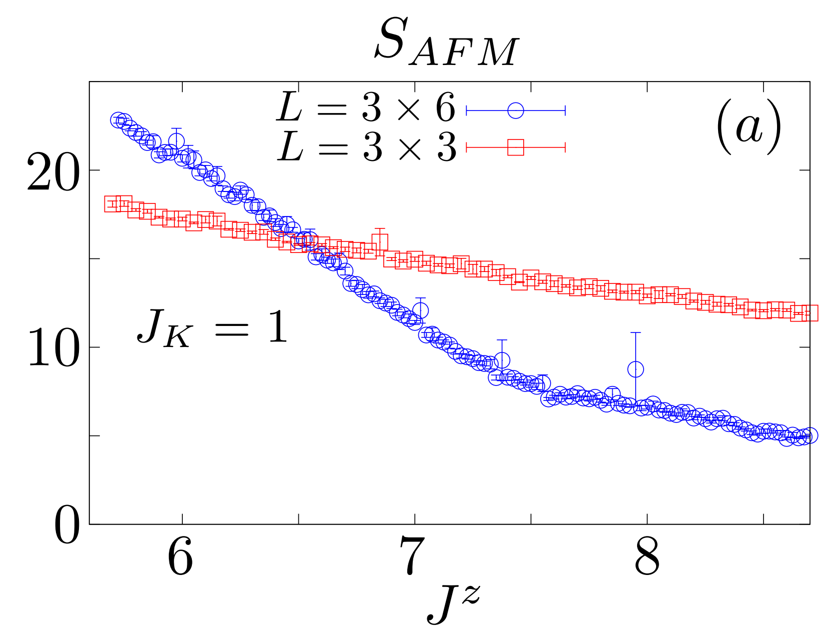




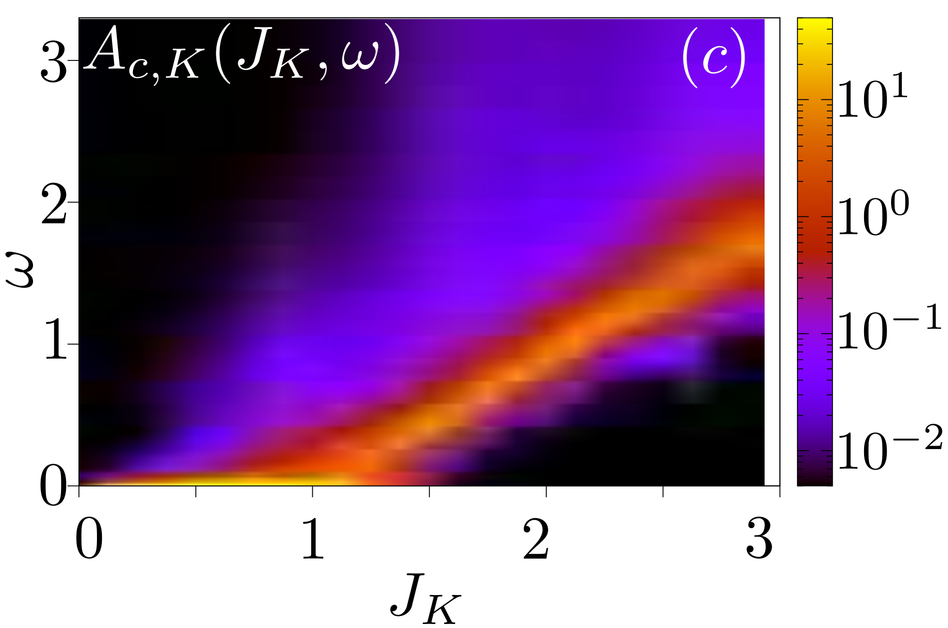


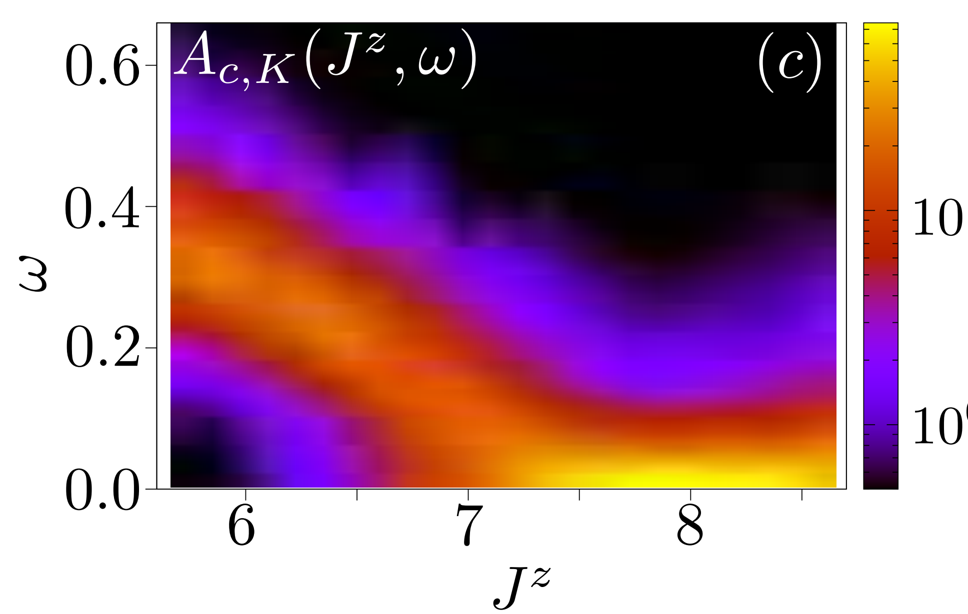
spin structure
factor





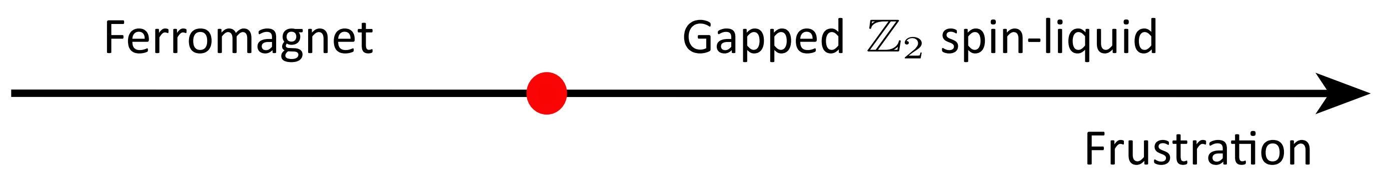
electron
spectral-fn.





Nature of Quantum Critical Point?

In the absence of conduction electrons,
the critical point is rather unconventional, and
has a rather large anomalous dimension.



$$\langle S^+(\vec{r},\tau)S^-(0,0)\rangle \sim \frac{1}{\left(r^2+\tau^2\right)^{1+\eta}}$$

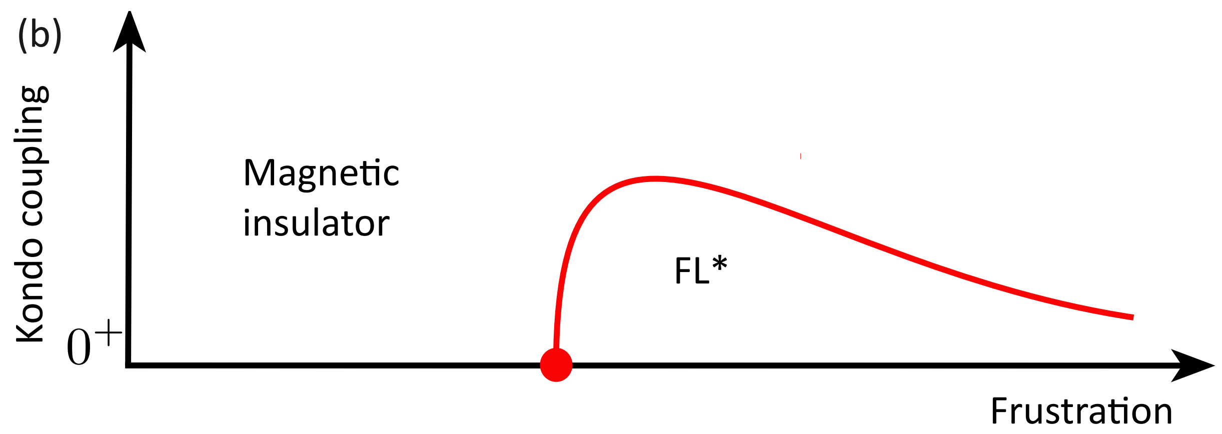
$$\eta \approx 1.37 > 1$$

(for Wilson-Fisher fixed point, $\eta \approx 0.03$)

[Chubukov, Senthil, Sachdev, 1994;
Isakov, Hastings, Melko, 2011]

Nature of Quantum Critical Point?

In the presence of conduction electrons,
Kondo coupling irrelevant at the transition
$\Rightarrow$ Kondo breakdown.



$$\frac{dJ_K}{dl} = (1 - \eta) J_K$$

Kondo coupling irrelevant at the critical point due to $\eta > 1$.

Critical magnetic fluctuations will show ω/T scaling.

[TG, Senthil 2010]

Summary and Questions

- Broad message: possible to construct sign-problem-free models that sometime allow unbiased simulation of strong correlation physics, e.g., Mott transition between superconductor and AFM on square lattice, non-Fermi liquids in certain Kondo systems, etc.

- Nodal superconductivity model as a starting point for DMRG to study doped phenomena e.g. pseudogap, strange metal etc.?

- Deconfined criticality between SC and AFM?

- Higher dimensional analogs of “mixed-dimension” Kondo lattice systems, e.g., 3d metal coupled to 2d local moments at or away from criticality?

- Detailed understanding of Kondo breakdown in Yb_2PT_2Pb?

- Sign problem forces us to think more deeply about the “sign structure” of many-body wavefunctions, which may be “universal” in a meaningful way.