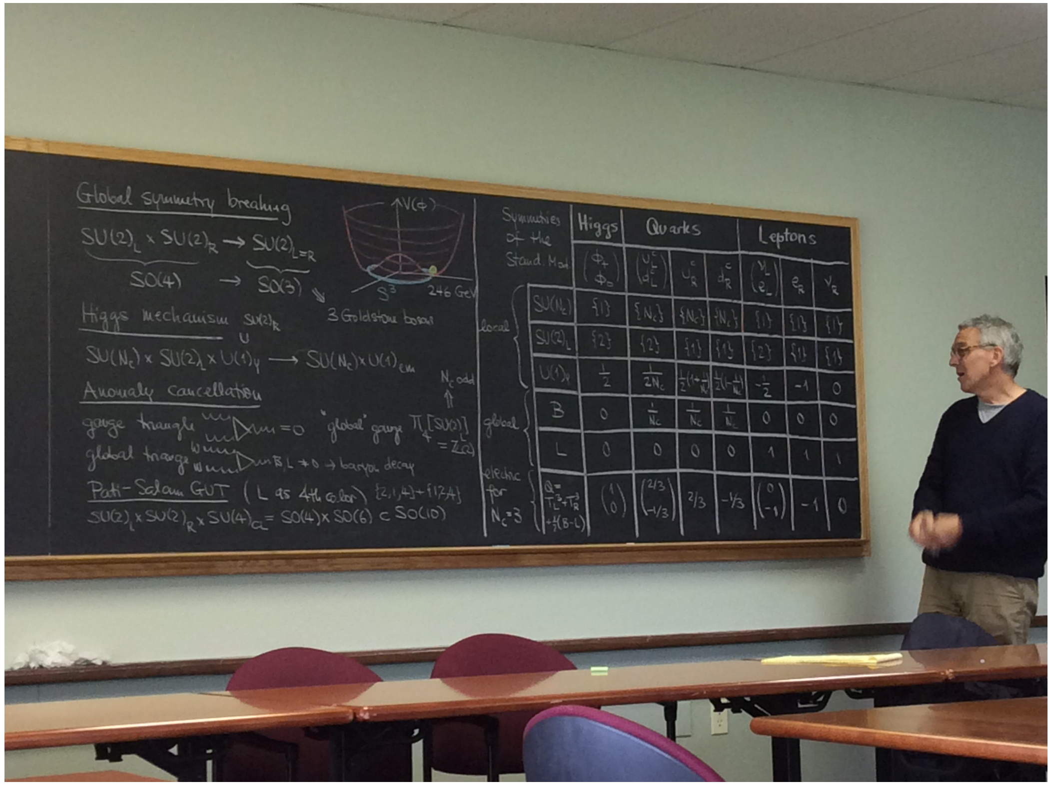
Julius-Maximilians-
UNIVERSITÄT
WÜRZBURG

Confronting the sign problem for frustrated magnets

Fakher F. Assaad, Workshop on the sign problem in QCD and beyond, Bern, January 20-24, 2025

Aspen, June, 2015



Thank you for promoting interdisciplinary research !

Julius-Maximilians-
UNIVERSITÄT
WÜRZBURG

Confronting the sign problem for frustrated magnets

Fakher F. Assaad, Workshop on the sign problem in QCD and beyond, Bern, January 20-24, 2025

Many phases of matter can be simulated with quantum Monte Carlo methods without encountering the sign problem!

Mott insulators, spin-liquids, Dirac systems, electron-phonon, spin systems with classical frustration, superconductors, quantum phase transitions, twisted bilayer graphene, continuum field theories...

S. Chandrasekharan and Uwe-Jens Wiese, Phys. Rev. Lett. 83 (1999).
C. Wu and S.-C. Zhang. Phys. Rev. B, 71, 155115, (2005).
E. Huffman and S. Chandrasekharan, Phys. Rev. B 89 (2014), 111101.
Zi-Xiang Li, Yi-Fan Jiang, and H. Yao Phys. Rev. Lett. 117 (2016), 267002.
Z. C. Wei, C. Wu, Yi Li, Shiwei Zhang, and T. Xiang. Phys. Rev. Lett. 116 (2016), 250601.

DFG
SFB1170
ToCoTronics
Q-M&S. Correlated Quantum Materials & Solid State Quantum Systems
Center of excellence – complexity and topology in quantum matter
NIC
lrz Leibniz-Rechenzentrum der Bayerischen Akademie der Wissenschaften
GCS Gauss Centre for Supercomputing
KONWIHR

Julius-Maximilians-UNIVERSITÄT WÜRZBURG

Confronting the sign problem for frustrated magnets

Fakher F. Assaad, Workshop on the sign problem in QCD and beyond, Bern, January 20-24 2025

Phases with sign problem include:

Frustrated magnets

PHYSICAL REVIEW B **104**, L081106 (2021)

Letter

Quantum Monte Carlo simulation of generalized Kitaev models

Toshihiro Sato[1] and Fakher F. Assaad[1,2]
[1]*Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany*
[2]*Würzburg-Dresden Cluster of Excellence ct.qmat, Am Hubland, 97074 Würzburg, Germany*

PHYSICAL REVIEW B **110**, L201114 (2024)

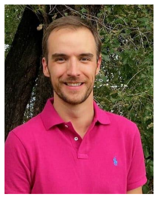
Letter

Scale-invariant magnetic anisotropy in α-$RuCl_3$: A quantum Monte Carlo study

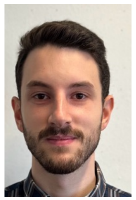
Toshihiro Sato,[1,2,3] B. J. Ramshaw,[4,5] K. A. Modic,[6] and Fakher F. Assaad[3,2]

T. Sato

K. Modic



B. Ramshaw



J. Inacio

Local moments in metallic environments

Z. Liu

B. Frank

M. Weber

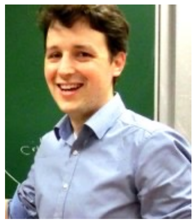
M. Raczkowski

B. Danu

S. Biswas

T. Grover

M. Vojta



L. Janssen

D. Luitz

Auxiliary field quantum Monte Carlo

$$Z = \mathrm{Tr} e^{-\beta \hat{H}} = \int D\left\{\Phi(i,\tau)\right\} e^{-S\left\{\Phi(i,\tau)\right\}}$$

$\Phi(\boldsymbol{x},\tau)$: Hubbard-Stratonovich (or arbitrary field with predefined dynamics)

Multidimensional integral → Monte Carlo

One body problem in external field → Polynomial complexity

R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D 24 (1981), 2278
J. E. Hirsch, Phys. Rev. B 31 (1985), 4403
White, D. Scalapino, R. Sugar, E. Loh, J. Gubernatis, and R. Scalettar, Phys. Rev. B 40 (1989), 506
....

Let $\hat{H} = \hat{H}_0 - \lambda \sum_n \left(\hat{\boldsymbol{c}}^\dagger O^{(n)} \hat{\boldsymbol{c}} \right)^2$ with $O^{(n)} = O^{(n),\dagger}$

Trotter

$$e^{-\beta \hat{H}} = \prod_{\tau=1}^{L_\tau} \left(e^{-\Delta\tau \hat{H}_0} \prod_n e^{\Delta\tau\lambda \left(\hat{\boldsymbol{c}}^\dagger O^{(n)} \hat{\boldsymbol{c}} \right)^2} \right) + \mathcal{O}\left(\Delta\tau\right)$$

$$L_\tau \Delta\tau = \beta$$

Hubbard-Stratonovich

$$e^{\hat{A}^2} = \frac{1}{\sqrt{2\pi}} \int d\Phi e^{-\frac{\Phi^2}{2} - \sqrt{2}\Phi \hat{A}}$$

$$e^{-S(\Phi(n,\tau))} \simeq e^{-\sum_{n,\tau} \Phi^2(n,\tau)/2} \,\mathrm{Tr} \prod_{\tau=1}^{L_\tau} \left(e^{-\Delta\tau \hat{H}_0} \prod_n e^{\sqrt{2\Delta\tau\lambda}\Phi(n,\tau) \hat{\boldsymbol{c}}^\dagger O^{(n)} \hat{\boldsymbol{c}}} \right) = e^{-\sum_{n,\tau} \Phi^2(n,\tau)/2 + \log \det M(\Phi)}$$

$$Z = \mathrm{Tr} e^{-\beta \hat{H}} = \int D\{\Phi(i,\tau)\} e^{-S\{\Phi(i,\tau)\}}$$

$$S\{\Phi\} = S_B\{\Phi\} - \log|\det(M\{\Phi\})| - i \arg\det M\{\Phi\}$$

$\arg\det M\{\Phi\} = 0$ No sign problem $\mathrm{CPU} \propto V^3 \beta$

$\arg\det M\{\Phi\} \in]0, 2\pi]$ Sign problem $\mathrm{CPU} \propto e^{2\alpha V \beta}$

Sample $\overline{S\{\Phi\}} = S_B\{\Phi\} - \log|\det(M\{\Phi\})|$

Compensate $\langle \mathrm{sign} \rangle = \dfrac{\int D\{\Phi(i,\tau)\} e^{-S\{\Phi\}}}{\int D\{\Phi(i,\tau)\} e^{-\overline{S\{\Phi\}}}} \propto e^{-\alpha\beta V}$

$$Z = \mathrm{Tr} e^{-\beta \hat{H}} = \int D\{\Phi(i,\tau)\} e^{-S\{\Phi(i,\tau)\}}$$

$$S\{\Phi\} = S_B\{\Phi\} - \log|\det(M\{\Phi\})| - i \arg\det M\{\Phi\}$$

$\arg\det M\{\Phi\} = 0$ No sign problem $\mathrm{CPU} \propto V^3\beta$

$\arg\det M\{\Phi\} \in]0, 2\pi]$ Sign problem $\mathrm{CPU} \propto e^{2\alpha V\beta}$

Sample $\overline{S\{\Phi\}} = S_B\{\Phi\} - \log|\det(M\{\Phi\})|$

Compensate $\langle \mathrm{sign} \rangle = \frac{\int D\{\Phi(i,\tau)\} e^{-S\{\Phi\}}}{\int D\{\Phi(i,\tau)\} e^{-\overline{S\{\Phi\}}}} \propto e^{-\alpha\beta V}$

This contribution:

Optimal formulations that minimize α so as to reach *interesting* energy scales

Designer models that avoid the sign problem but retain aspects of the physics one wishes to study.

Julius-Maximilians-
UNIVERSITÄT WÜRZBURG

Algorithms for Lattice fermions @ http://alf.physik.uni-wuerzburg.de/

ALF 1.0: SciPost Phys. 3 (2017), 013   ALF 2.0 SciPost Phys. Codebases 1 (2022)

Kinetic

Potential (sum of perfect squares)

$$\hat{H} = \sum_{k=1}^{M_T}\sum_{\sigma=1}^{N_{\rm col}}\sum_{s=1}^{N_{\rm fl}}\sum_{x,y}^{N_{\rm dim}} \hat{c}^{\dagger}_{x\sigma s} T^{(ks)}_{xy}\hat{c}_{y\sigma s} + \sum_{k=1}^{M_V} U_k \left\{ \sum_{\sigma=1}^{N_{\rm col}}\sum_{s=1}^{N_{\rm fl}} \left[\left(\sum_{x,y}^{N_{\rm dim}} \hat{c}^{\dagger}_{x\sigma s} V^{(ks)}_{xy}\hat{c}_{y\sigma s} \right) + \alpha_{ks} \right] \right\}^2$$

Coupling of fermions to bosonic fields with predefined dynamics

$$+ \sum_{k=1}^{M_I} \hat{Z}_k \left(\sum_{\sigma=1}^{N_{\rm col}}\sum_{s=1}^{N_{\rm fl}}\sum_{x,y}^{N_{\rm dim}} \hat{c}^{\dagger}_{x\sigma s} I^{(ks)}_{xy}\hat{c}_{y\sigma s} \right) + \hat{H}_{\rm Ising}$$

- Block diagonal in flavors, $N_{\rm fl}$
- SU($N_{\rm col}$) symmetric in colors $N_{\rm col}$
- Arbitrary Bravais lattice for d=1,2
- Model can be specified at minimal programming cost
- Fortran 2008 standard
- MPI implementation
- Global and local moves, Parallel tempering, Langevin, HMC
- Projective and finite T approaches
- pyALF: easy access python interface
- Predefined models


F. Goth


M. Bercx


J. Hoffmann


J. S.E. Portela


J. Schwab


Z. Liu


E. Huffman


A. Götz


F. Parisen Toldin

DFG Wissenschaftliche Literaturversorgungs und Informationssysteme (LIS)

KONWIHR

Confronting the sign problem for frustrated magnets

Fakher F. Assaad, Workshop on the sign problem in QCD and beyond, Bern, January 20-24 2025

Phases with sign problem include:

Frustrated magnets

PHYSICAL REVIEW B **104**, L081106 (2021)

Letter

Quantum Monte Carlo simulation of generalized Kitaev models

Toshihiro Sato[1] and Fakher F. Assaad[1,2]

[1]*Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany*
[2]*Würzburg-Dresden Cluster of Excellence ct.qmat, Am Hubland, 97074 Würzburg, Germany*

PHYSICAL REVIEW B **110**, L201114 (2024)

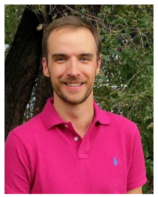
Letter

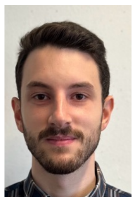
Scale-invariant magnetic anisotropy in α-$RuCl_3$: A quantum Monte Carlo study

Toshihiro Sato,[1,2,3] B. J. Ramshaw,[4,5] K. A. Modic,[6] and Fakher F. Assaad[3,2]


T. Sato


K. Modic


B. Ramshaw


J. Inacio

Local moments in metallic environments


Z. Liu


B. Frank


M. Weber

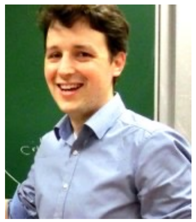

M. Raczkowski


B. Danu


S. Biswas

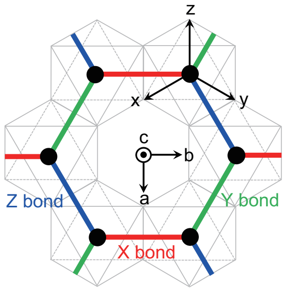

T. Grover


M. Vojta


L. Janssen


D. Luitz

Confronting the sign problem for frustrated magnets

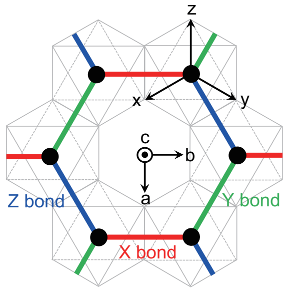


$$\hat{H} = 2K \sum_{i \in A, \delta} \hat{S}_i^{\delta} \hat{S}_{i+\delta}^{\delta} + J \sum_{i \in A, \boldsymbol{\delta}} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+\delta}.$$

A. Kitaev, Annals of Physics 321 (2006), no. 1 2 – 111.

$$K = A\sin(\varphi), \;\; J = A\cos(\varphi), \;\; A = \sqrt{K^2 + J^2}$$

Confronting the sign problem for frustrated magnets



$$\hat{H} = 2K \sum_{i\in A,\delta} \hat{S}_i^{\delta}\hat{S}_{i+\delta}^{\delta} + J \sum_{i\in A,\boldsymbol{\delta}} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+\delta}.$$

$$K = A\sin(\varphi),\;\; J = A\cos(\varphi),\;\; A = \sqrt{K^2+J^2}$$

<u>Simulating spins with fermions.</u>

$$\hat{S}_i^{\delta} = \frac{1}{2}\sum_{s,s'} \hat{f}_{i,s}^{\dagger}\sigma_{s,s'}^{\delta}\hat{f}_{i,s'}$$

$$\sum_s \hat{f}_{i,s}^{\dagger}\hat{f}_{i,s} \equiv \hat{n}_i = 1$$

$$\hat{H}_{QMC} = |K| \sum_{i\in A,\delta} s_\delta \left(s_\delta \hat{S}_i^{\delta} + \frac{K}{|K|}\hat{S}_{i+\delta}^{\delta} \right)^2 - \frac{J}{8}\sum_{i\in A,\delta}\left(\left[\hat{D}_{i,\delta}^{\dagger} + \hat{D}_{i,\delta}\right]^2 + \left[i\hat{D}_{i,\delta} - i\hat{D}_{i,\delta}^{\dagger}\right]^2 \right) + U\sum_i (\hat{n}_i - 1)^2$$

$$\hat{D}_{i,\delta}^{\dagger} = \sum_s \hat{f}_{i,s}^{\dagger}\hat{f}_{i+\delta,s}$$

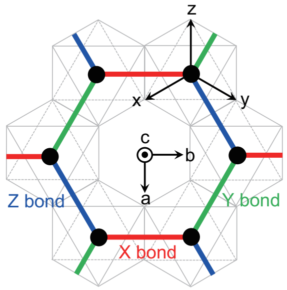
$$s_\delta = \pm 1$$

$$\hat{H}_{QMC}\Big|_{(-1)^{\hat{n}_i}=-1} = \hat{H} + C \quad \forall\, s_\delta = \pm 1$$

Constraint commutes with Hamiltonian dynamics

$$\left[\hat{H}_{QMC}, (-1)^{\hat{n}_i}\right] = 0$$

Confronting the sign problem for frustrated magnets

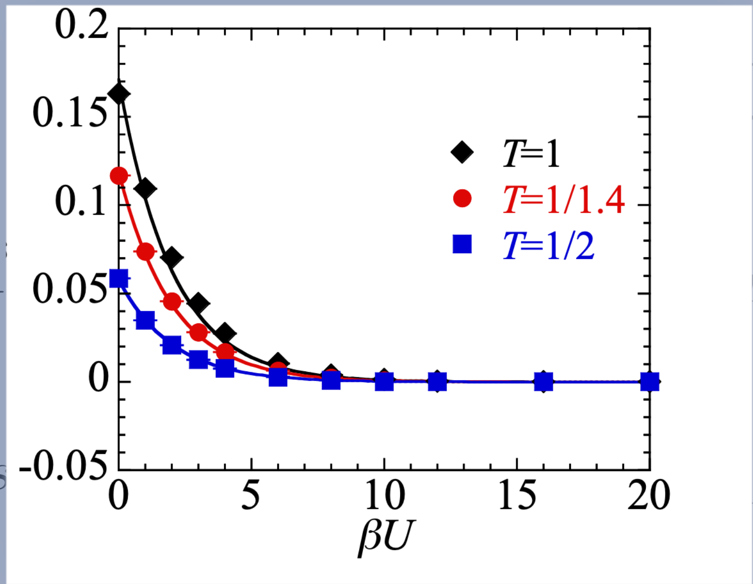


$$\hat{H} = 2K \sum_{i \in A, \delta} \hat{S}_i^{\delta} \hat{S}_{i+\delta}^{\delta} + J \sum_{i \in A, \boldsymbol{\delta}} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+\delta}.$$

$$K = A\sin(\varphi), \;\; J = A\cos(\varphi), \;\; A = \sqrt{K^2 + J^2}$$

Simulating spins with fermions.

$$\sum \hat{f}_{i,s}^{\dagger} \hat{f}_{i,s} \equiv \hat{n}_i = 1$$



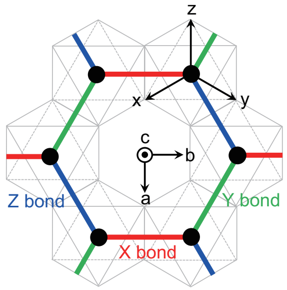
$$\hat{H}_{QMC} = |K| \sum_{i \in A, \delta} s_{\delta} \Big(s_{\delta} \hat{S}_i^{\delta} + \; \cdots \; \hat{D}_{i,\delta} - i\hat{D}_{i,\delta}^{\dagger} \Big]^2 \Big) + U \sum_i (\hat{n}_i - 1)^2$$

$$\hat{D}_{i,\delta}^{\dagger} = \sum_s \hat{f}_{i,s}^{\dagger} \hat{f}_{i+\delta,s}$$

$$\cdots = \hat{H} + C \qquad \forall\, s_{\delta} = \pm 1$$

Constraint commutes with Hamiltonian dynamics $\left[\hat{H}_{QMC}, (-1)^{\hat{n}_i}\right] = 0$

Confronting the sign problem for frustrated magnets



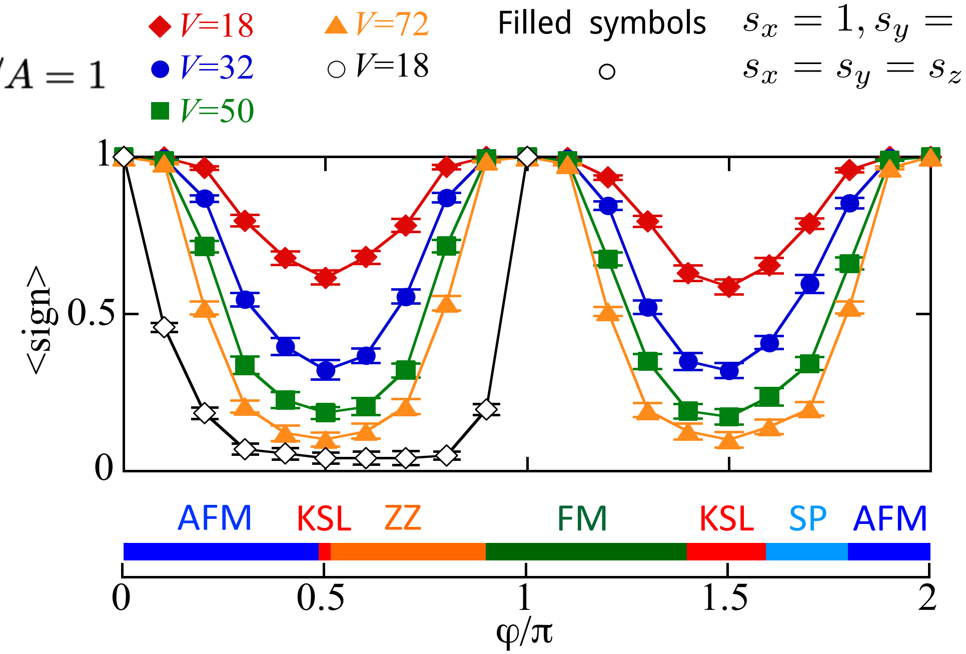
$$\hat{H} = 2K \sum_{i\in A,\delta} \hat{S}_i^{\delta} \hat{S}_{i+\delta}^{\delta} + J \sum_{i\in A,\boldsymbol{\delta}} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+\delta}.$$

$$K = A\sin(\varphi),\ J = A\cos(\varphi),\ A = \sqrt{K^2 + J^2}$$

$T/A = 1$

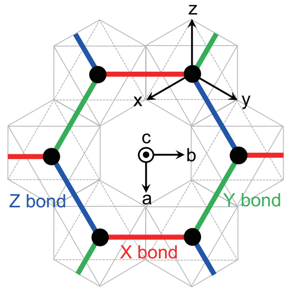
Filled symbols $s_x = 1, s_y = s_z = -1$

○ $s_x = s_y = s_z = 1$



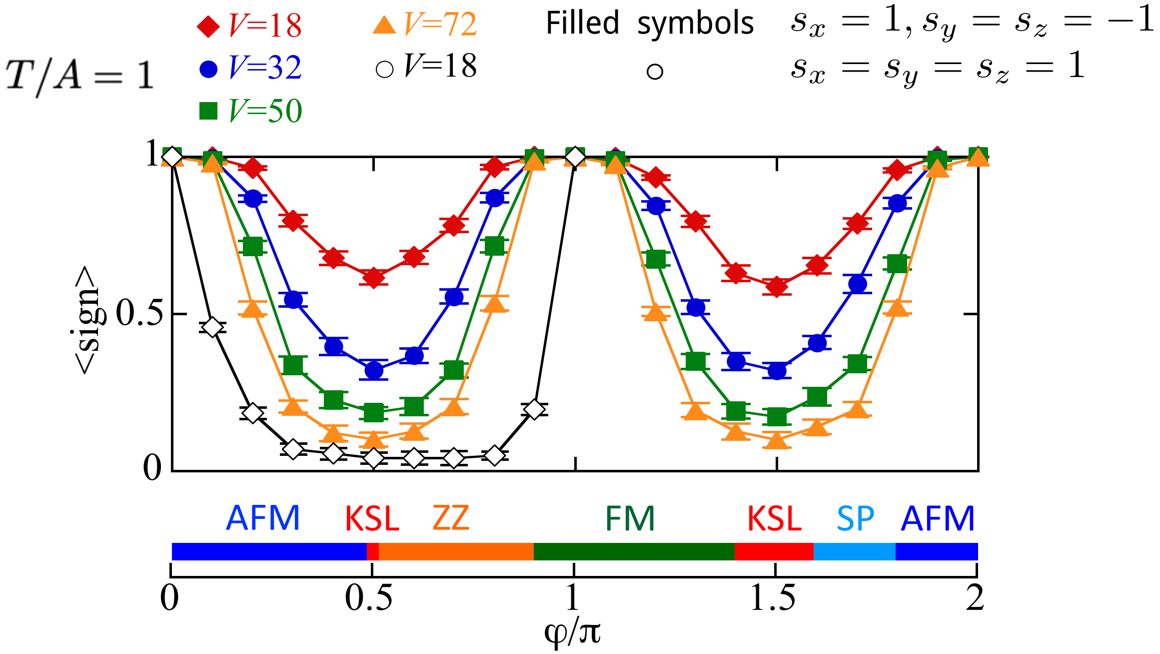
J. Chaloupka, G. Jackeli, and G.Khaliullin Phys. Rev. Lett. 105 (2010), 027204.

Confronting the sign problem for frustrated magnets

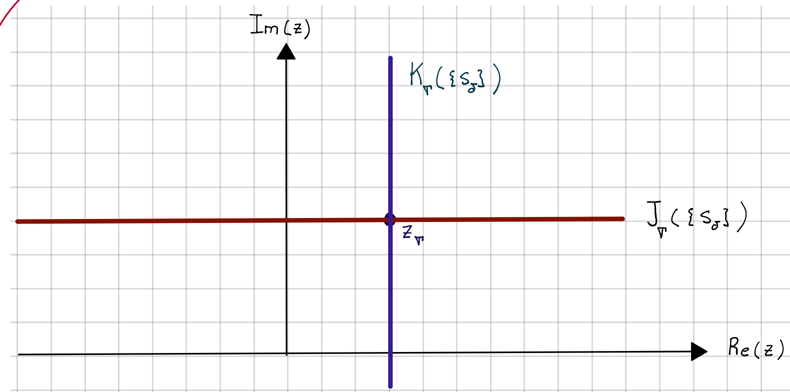


$$\hat{H} = 2K \sum_{i\in A,\delta} \hat{S}_i^{\delta} \hat{S}_{i+\delta}^{\delta} + J \sum_{i\in A,\boldsymbol{\delta}} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+\delta}.$$

$$K = A\sin(\varphi),\;\; J = A\cos(\varphi),\;\; A = \sqrt{K^2 + J^2}$$

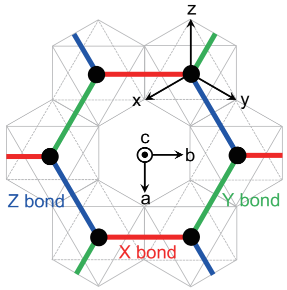


J. Chaloupka, G. Jackeli, and G.Khaliullin Phys. Rev. Lett. 105 (2010), 027204.



Complex saddle points and thimbles depend upon the gauge choice $\{s_\delta\}$. Optimal gauge choice minimizes the distance from the dominant saddle point to the real axis.

Confronting the sign problem for frustrated magnets



$$\hat{H} = 2K \sum_{i \in A, \delta} \hat{S}_i^{\delta} \hat{S}_{i+\delta}^{\delta} + J \sum_{i \in A, \boldsymbol{\delta}} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+\delta}.$$

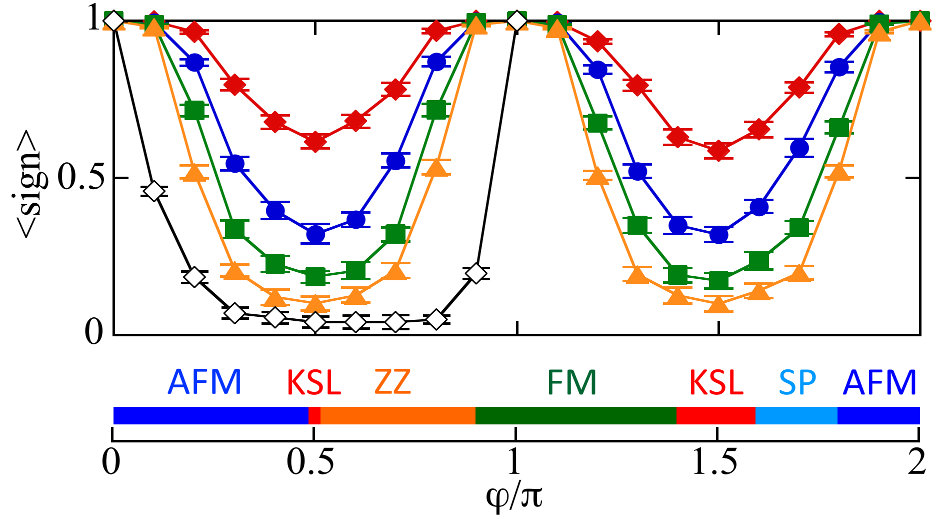
$$K = A\sin(\varphi), \;\; J = A\cos(\varphi), \;\; A = \sqrt{K^2 + J^2}$$

$T/A = 1$

◆ V=18 ▲ V=72 Filled symbols $s_x = 1, s_y = s_z = -1$

● V=32 ○ V=18 ○ $s_x = s_y = s_z = 1$

■ V=50



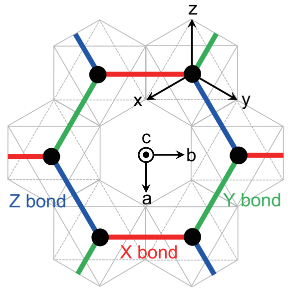
Possible to reach temperatures down to $\beta A \simeq 3$

$A \simeq 10meV \simeq 100K$

→ Experimentally relevant energy scales are accessible

J. Chaloupka, G. Jackeli, and G.Khaliullin Phys. Rev. Lett. 105 (2010), 027204.

Confronting the sign problem for frustrated magnets



$$\hat{H} = 2K \sum_{i \in A, \delta} \hat{S}_i^{\delta} \hat{S}_{i+\delta}^{\delta} + J \sum_{i \in A, \boldsymbol{\delta}} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+\delta}.$$

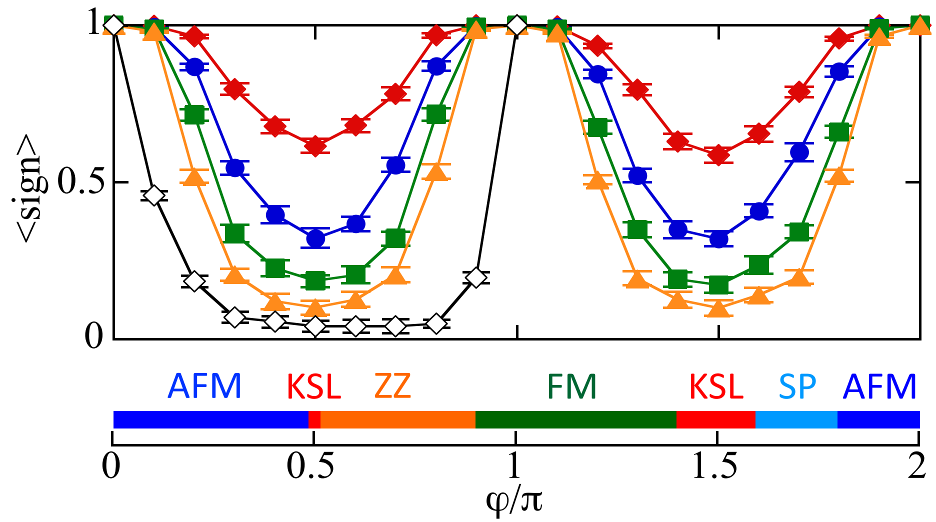
$$K = A\sin(\varphi), \; J = A\cos(\varphi), \; A = \sqrt{K^2 + J^2}$$

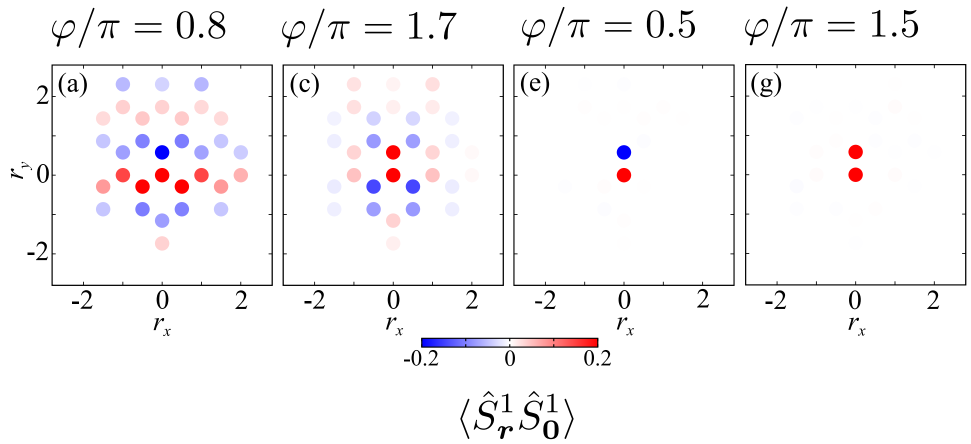
$T/A = 1$

◆ V=18 ▲ V=72
● V=32 ○ V=18
■ V=50

Filled symbols $s_x = 1, s_y = s_z = -1$

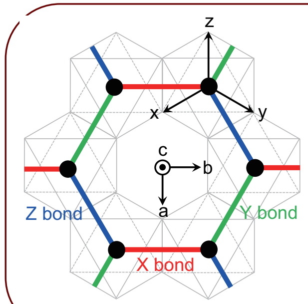
○ $s_x = s_y = s_z = 1$





J. Chaloupka, G. Jackeli, and G.Khaliullin Phys. Rev. Lett. 105 (2010), 027204.

Confronting the sign problem for frustrated magnets



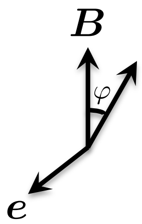
$RuCl_3$

$$\hat{H}(\varphi) = \sum_{\langle i,j\rangle}\left[K\hat{S}_i^{\gamma}\hat{S}_j^{\gamma} + \Gamma\hat{S}_i^{\alpha}\hat{S}_j^{\beta} + J_1\hat{\boldsymbol{S}}_i\cdot\hat{\boldsymbol{S}}_j\right] + J_3\sum_{\langle\langle i,j\rangle\rangle}\hat{\boldsymbol{S}}_i\cdot\hat{\boldsymbol{S}}_j - \mu_B\sum_i \boldsymbol{B}(\varphi)\cdot\boldsymbol{g}\hat{\boldsymbol{S}}_i$$

$$(J_1, J_3, K, \Gamma) = (-0.5, 0.5, -5.0, 2.5)\ [\mathrm{meV}] \qquad \boldsymbol{g} = \mathrm{diag}\,[2.3, 2.3, 1.3]$$

Winter et al. Nat. Comm. 8 (2017), PRL. 120 (2018)

Magnetic rigidity: magnetotropic susceptibility

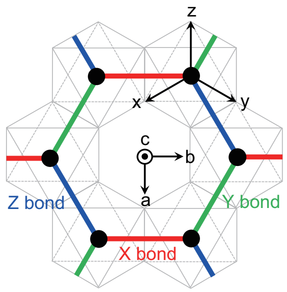


$$e^{i\varphi\boldsymbol{K}\cdot\boldsymbol{e}}\boldsymbol{B} \equiv \boldsymbol{B}(\varphi)$$

$$k \equiv \left.\frac{\partial^2 F(\varphi)}{\partial\varphi^2}\right|_{\varphi=0} = \mu_B\boldsymbol{g}\langle\hat{\boldsymbol{S}}_{tot}\rangle\cdot\boldsymbol{e}\times(\boldsymbol{e}\times\boldsymbol{B})$$

$$-\mu_B^2\int_0^{\beta} d\tau\left[\langle\left(\boldsymbol{g}\hat{\boldsymbol{S}}_{tot}(\tau)\cdot\boldsymbol{e}\times\boldsymbol{B}\right)\left(\boldsymbol{g}\hat{\boldsymbol{S}}_{tot}(0)\cdot\boldsymbol{e}\times\boldsymbol{B}\right)\rangle - \left(\langle\boldsymbol{g}\hat{\boldsymbol{S}}_{tot}(0)\cdot\boldsymbol{e}\times\boldsymbol{B}\rangle\right)^2\right]$$

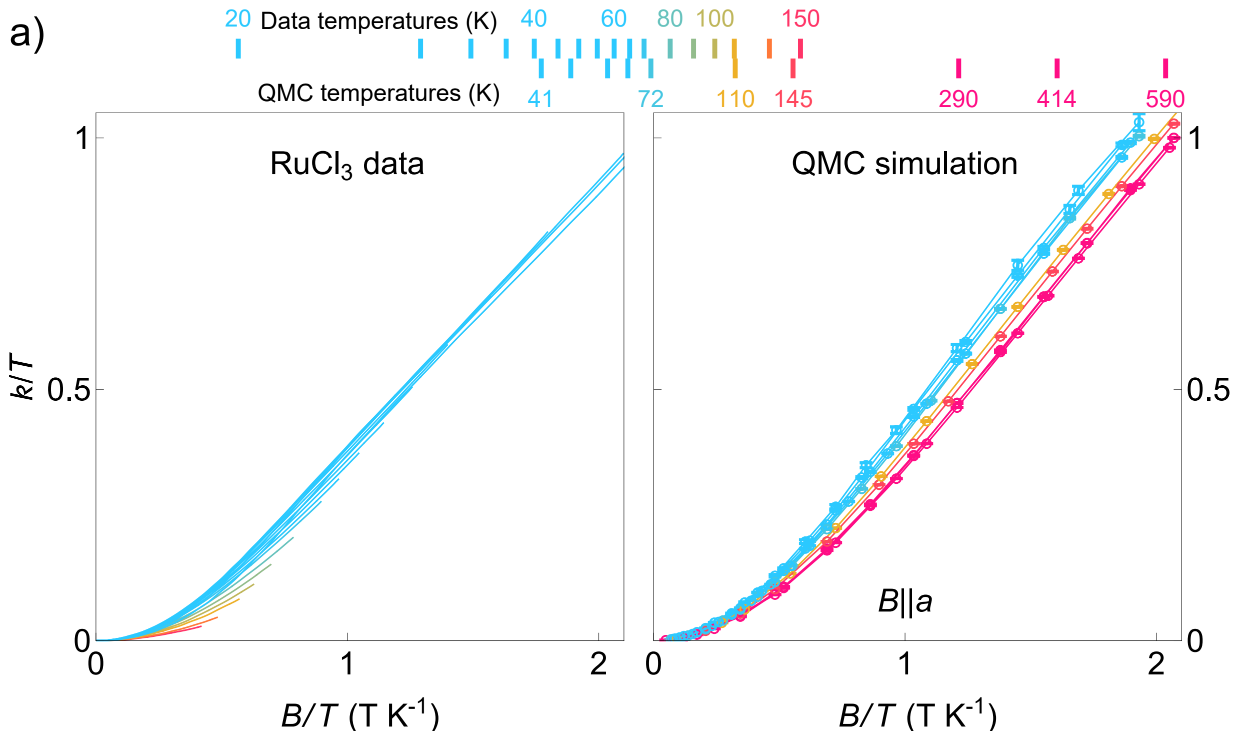
Confronting the sign problem for frustrated magnets



ARTICLES
https://doi.org/10.1038/s41567-020-1028-0
nature physics
Check for updates

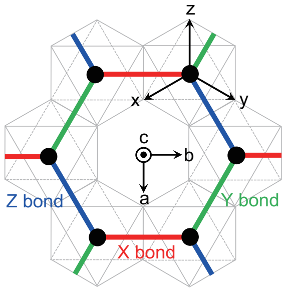
Scale-invariant magnetic anisotropy in $RuCl_3$ at high magnetic fields

K. A. Modic[1,2], Ross D. McDonald[3], J. P. C. Ruff[4], Maja D. Bachmann[2,5], You Lai[3,6,7], Johanna C. Palmstrom[5], David Graf[7], Mun K. Chan[3], F. F. Balakirev[3], J. B. Betts[3], G. S. Boebinger[6,7], Marcus Schmidt[2], Michael J. Lawler[8], D. A. Sokolov[2], Philip J. W. Moll[2,9], B. J. Ramshaw[8] and Arkady Shekhter[7]



For a local moment: $$\frac{k}{T} = f(B/T)$$

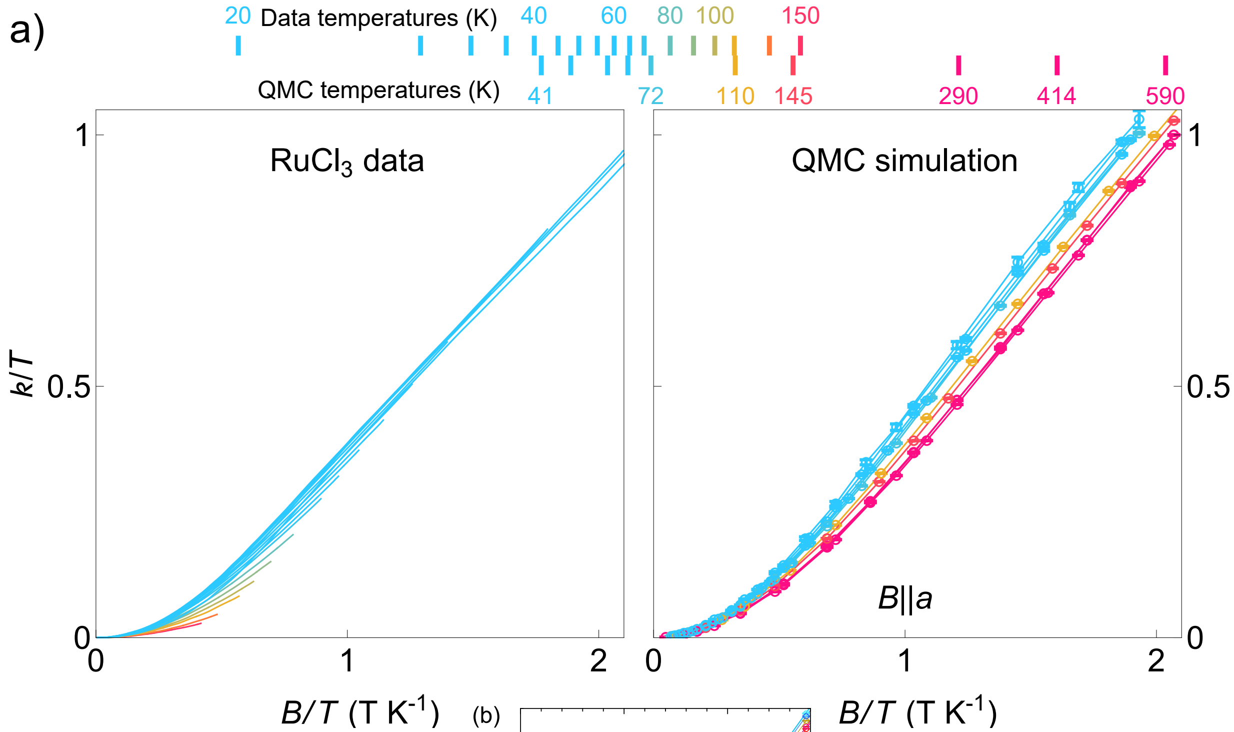
Confronting the sign problem for frustrated magnets



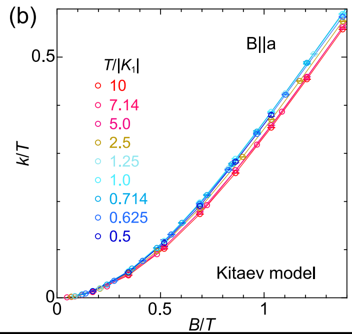
ARTICLES
https://doi.org/10.1038/s41567-020-1028-0
nature physics
Check for updates

Scale-invariant magnetic anisotropy in $RuCl_3$ at high magnetic fields

K. A. Modic[1,2], Ross D. McDonald[3], J. P. C. Ruff[4], Maja D. Bachmann[2,5], You Lai[3,6,7], Johanna C. Palmstrom[5], David Graf[7], Mun K. Chan[3], F. F. Balakirev[3], J. B. Betts[3], G. S. Boebinger[6,7], Marcus Schmidt[2], Michael J. Lawler[8], D. A. Sokolov[2], Philip J. W. Moll[2,9], B. J. Ramshaw[8] and Arkady Shekhter[7]



For a local moment: $$\frac{k}{T} = f(B/T)$$



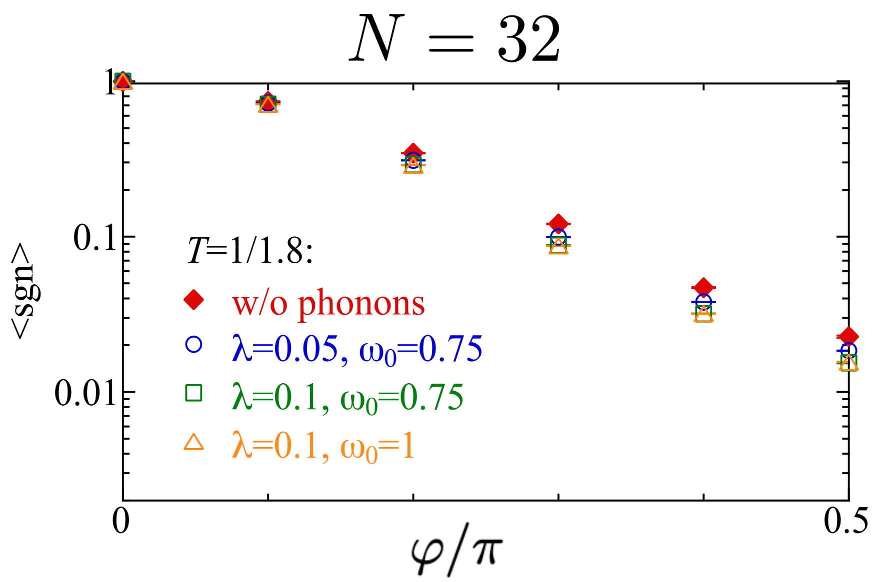
Pure Kitaev model

Confronting the sign problem for frustrated magnets

Next steps? Debye temperature ~ 200K Magnetic energy scale ~ 100K

$$\hat{H} = \sum_{b=[i\in A,\delta]} \frac{\hat{P}_b^2}{2m} + \frac{k}{2}\hat{Q}_b + 2K(1+\hat{Q}_b)\hat{S}_i^{\delta}\hat{S}_{i+\delta}^{\delta} + J(1+\hat{Q}_b)\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+\delta}$$

$$\omega_0 = \sqrt{\frac{k}{m}}, \quad \lambda = \frac{1}{2k}$$



Coupling to phonons does not lead to a more severe sign problem!

$$K = A\sin(\varphi), \ J = A\cos(\varphi), \ A = \sqrt{K^2 + J^2}$$

Confronting the sign problem for frustrated magnets

Fakher F. Assaad, Workshop on the sign problem in QCD and beyond, Bern, January 20-24, 2025

Summary (I)

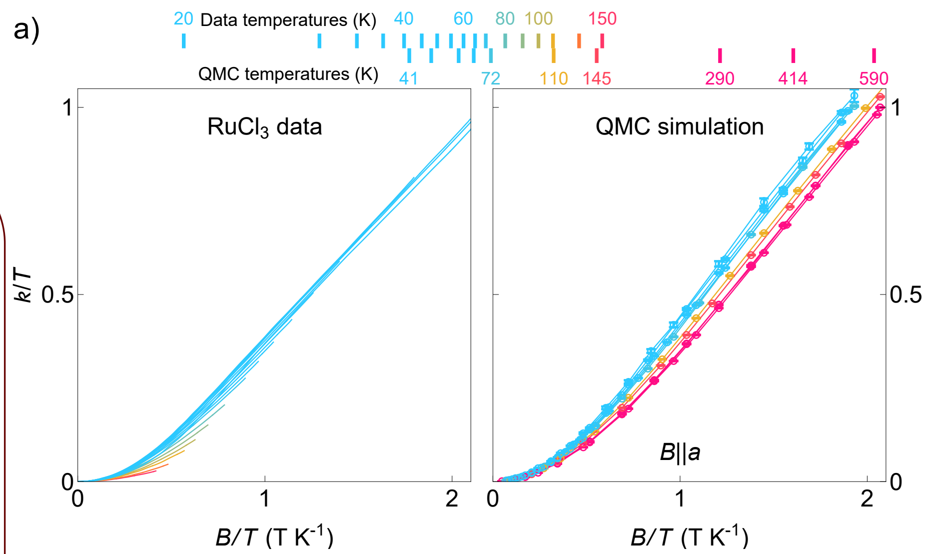
$$Z = \mathrm{Tr} e^{-\beta \hat{H}} = \int D\left\{\Phi(i,\tau)\right\} e^{-S\{\Phi(i,\tau)\}}$$

We can simulate models of Kitaev materials down to experimentally relevant energy scales.

Tool to determine model parameters.

Coupling to phonons does not render the sign problem more severe.

There may be room for improvement: $2^3 \rightarrow 2^{3N}$ gauge variables.



Confronting the sign problem for frustrated magnets

Fakher F. Assaad, Workshop on the sign problem in QCD and beyond, Bern, January 20-24 2025

Phases with sign problem include:

Frustrated magnets

PHYSICAL REVIEW B **104**, L081106 (2021)

Letter

Quantum Monte Carlo simulation of generalized Kitaev models

Toshihiro Sato[1] and Fakher F. Assaad[1,2]
[1] *Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany*
[2] *Würzburg-Dresden Cluster of Excellence ct.qmat, Am Hubland, 97074 Würzburg, Germany*

PHYSICAL REVIEW B **110**, L201114 (2024)

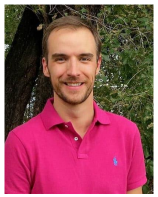
Letter

Scale-invariant magnetic anisotropy in α-RuCl$_3$: A quantum Monte Carlo study

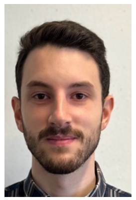
Toshihiro Sato,[1,2,3] B. J. Ramshaw,[4,5] K. A. Modic,[6] and Fakher F. Assaad[3,2]

T. Sato

K. Modic



B. Ramshaw



J. Inacio

Local moments in metallic environments

Z. Liu

B. Frank

M. Weber

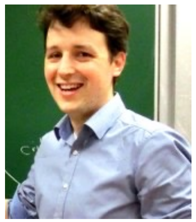
M. Raczkowski

B. Danu

S. Biswas

T. Grover

M. Vojta



L. Janssen

D. Luitz

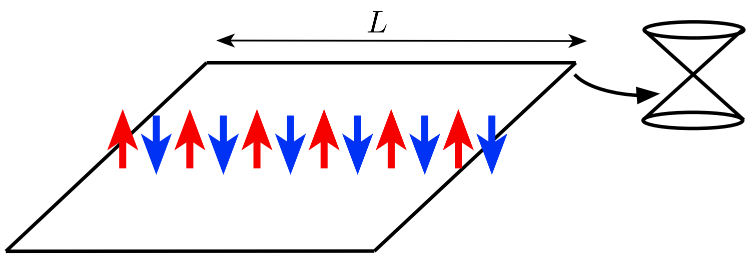
Local moments in metals

A local moment is generated by a repulsive Hubbard term that localizes a single electron without breaking spin rotational symmetry:

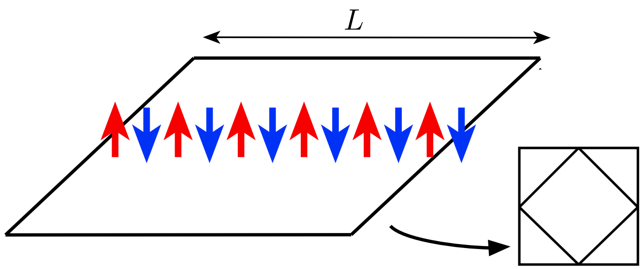
$$U\left(\hat{n}_r - 1\right)^2$$

Particle-hole symmetry is required to avoid the negative sign problem. For a **dense** number of local moments this invariably leads to an antiferromagnetic instability and an insulating state.

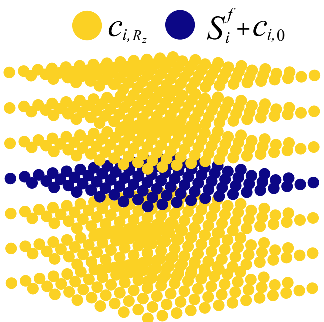
Local moments in metals



Dimensional mismatch Kondo systems



$$\hat{H} = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} (\hat{\boldsymbol{c}}_{\boldsymbol{i}}^{\dagger} \hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) + \frac{J_k}{2} \sum_{\boldsymbol{r}} \hat{\boldsymbol{c}}_{\boldsymbol{r}}^{\dagger} \boldsymbol{\sigma} \hat{\boldsymbol{c}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}} + J_h \sum_{\langle \boldsymbol{r},\boldsymbol{r}' \rangle} \hat{\boldsymbol{S}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}'}$$



Magnetic impurities are sub-intensive

System remains metallic even at particle-hole symmetry

Local moments in metals

$$\hat{H} = -t\sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle}(\hat{\boldsymbol{c}}_{\boldsymbol{i}}^{\dagger}\hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) + \frac{J_k}{2}\sum_{\boldsymbol{r}}\hat{\boldsymbol{c}}_{\boldsymbol{r}}^{\dagger}\boldsymbol{\sigma}\hat{\boldsymbol{c}}_{\boldsymbol{r}}\cdot\hat{\boldsymbol{S}}_{\boldsymbol{r}} + J_h\sum_{\langle \boldsymbol{r},\boldsymbol{r}'\rangle}\hat{\boldsymbol{S}}_{\boldsymbol{r}}\cdot\hat{\boldsymbol{S}}_{\boldsymbol{r}'}$$

Field theory: $\hat{\boldsymbol{S}}_{\boldsymbol{r}} = \frac{1}{2}\hat{\boldsymbol{f}}_{\boldsymbol{r}}^{\dagger}\boldsymbol{\sigma}\hat{\boldsymbol{f}}_{\boldsymbol{r}}$ with constraint $\hat{\boldsymbol{f}}_{\boldsymbol{r}}^{\dagger}\hat{\boldsymbol{f}}_{\boldsymbol{r}} = 1$ Def $\hat{\boldsymbol{f}}_{\boldsymbol{r}}^{\dagger} = \left(\hat{f}_{\boldsymbol{r},\uparrow}^{\dagger}, \hat{f}_{\boldsymbol{r},\downarrow}^{\dagger}\right)$

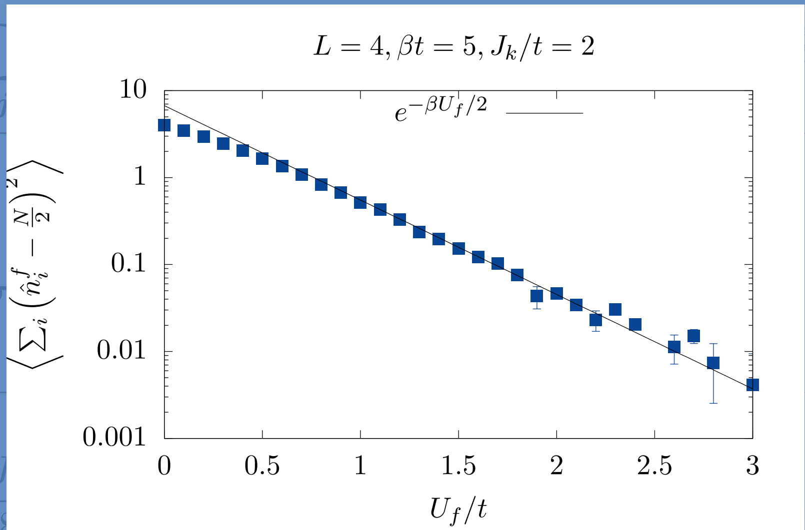
$$\hat{H} = -t\sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle}(\hat{\boldsymbol{c}}_{\boldsymbol{i}}^{\dagger}\hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) - \frac{J_k}{8}\sum_{\boldsymbol{r}}\left[\left(\hat{V}_{\boldsymbol{r}} + \hat{V}_{\boldsymbol{r}}^{\dagger}\right)^2 + \left(i\hat{V}_{\boldsymbol{r}} - i\hat{V}_{\boldsymbol{r}}^{\dagger}\right)^2\right]$$
$$- \frac{J_h}{8}\sum_{b=\langle \boldsymbol{r},\boldsymbol{r}'\rangle}\left[\left(\hat{D}_b + \hat{D}_b^{\dagger}\right)^2 + \left(i\hat{D}_b - i\hat{D}_b^{\dagger}\right)^2\right] + \underbrace{U\sum_{\boldsymbol{r}}\left(\hat{\boldsymbol{f}}_{\boldsymbol{r}}^{\dagger}\hat{\boldsymbol{f}}_{\boldsymbol{r}} - 1\right)^2}_{=\hat{H}_U}$$

$\hat{D}_b = \hat{\boldsymbol{f}}_{\boldsymbol{r}}^{\dagger}\hat{\boldsymbol{f}}_{\boldsymbol{r}'}, \quad \hat{V}_{\boldsymbol{r}} = \hat{\boldsymbol{f}}_{\boldsymbol{r}}^{\dagger}\hat{\boldsymbol{c}}_{\boldsymbol{r}}$

Exact in the limit $U \rightarrow \infty$. But since $\left[\hat{H}_U, \hat{H}\right] = 0$ the constraint is imposed very efficiently.

Local moments in metals

$$\hat{H} = -t \sum_{\langle i,j \rangle} \ldots \hat{\boldsymbol{S}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}'}$$



Field theory: $\hat{\boldsymbol{S}}_{\boldsymbol{r}} = \frac{1}{2} \hat{\boldsymbol{f}}^{\dagger}_{\boldsymbol{r}} \boldsymbol{\sigma} \ldots$ Def $\hat{\boldsymbol{f}}^{\dagger}_{\boldsymbol{r}} = \left(\hat{f}^{\dagger}_{\boldsymbol{r},\uparrow}, \hat{f}^{\dagger}_{\boldsymbol{r},\downarrow} \right)$

$$\hat{H} = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} (\hat{\boldsymbol{c}}^{\dagger}_{\boldsymbol{i}} \hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) - \frac{J}{8} \sum_{\boldsymbol{r}} \left[\ldots \right]$$

$$-\frac{J_h}{8} \sum_{b=\langle \boldsymbol{r},\boldsymbol{r}' \rangle} \left[\left(\hat{D}_b + \hat{D}_b^{\dagger} \right)^2 + \left(i\hat{D}_b - i\hat{D}_b^{\dagger} \right)^2 \right] + \underbrace{U \sum_{\boldsymbol{r}} \left(\hat{\boldsymbol{f}}^{\dagger}_{\boldsymbol{r}} \hat{\boldsymbol{f}}_{\boldsymbol{r}} - 1 \right)^2}_{= \hat{H}_U}$$

$\hat{D}_b = \hat{\boldsymbol{f}}^{\dagger}_{\boldsymbol{r}} \hat{\boldsymbol{f}}_{\boldsymbol{r}'}, \quad \hat{V}_{\boldsymbol{r}} = \hat{\boldsymbol{f}}^{\dagger}_{\boldsymbol{r}} \hat{\boldsymbol{c}}_{\boldsymbol{r}}$

Exact in the limit $U \to \infty$. But since $\left[\hat{H}_U, \hat{H} \right] = 0$ the constraint is imposed very efficiently.

Local moments in metals

$$b_{\boldsymbol{r}} = |b_{\boldsymbol{r}}| e^{i\varphi_{\boldsymbol{r}}}$$

$$\hat{H} = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} (\hat{\boldsymbol{c}}^{\dagger}_{\boldsymbol{i}} \hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) \quad - \frac{J_k}{8} \sum_{\boldsymbol{r}} \left[\left(\hat{V}_{\boldsymbol{r}} + \hat{V}^{\dagger}_{\boldsymbol{r}} \right)^2 + \left(i\hat{V}_{\boldsymbol{r}} - i\hat{V}^{\dagger}_{\boldsymbol{r}} \right)^2 \right]$$

$$- \frac{J_h}{8} \sum_{b = \langle \boldsymbol{r}, \boldsymbol{r}' \rangle} \left[\left(\hat{D}_b + \hat{D}^{\dagger}_b \right)^2 + \left(i\hat{D}_b - i\hat{D}^{\dagger}_b \right)^2 \right] + U \sum_{\boldsymbol{r}} \left(\hat{\boldsymbol{f}}^{\dagger}_{\boldsymbol{r}} \hat{\boldsymbol{f}}_{\boldsymbol{r}} - 1 \right)^2$$

$$\hat{D}_b = \hat{\boldsymbol{f}}^{\dagger}_{\boldsymbol{r}} \hat{\boldsymbol{f}}_{\boldsymbol{r}'}, \quad \hat{V}_{\boldsymbol{r}} = \hat{\boldsymbol{f}}^{\dagger}_{\boldsymbol{r}} \hat{\boldsymbol{c}}_{\boldsymbol{r}} \qquad \chi_b = |\chi_b| e^{i \int_{\boldsymbol{r}}^{\boldsymbol{r}'} \boldsymbol{a} \cdot d\boldsymbol{l}} \qquad a_0$$

Partition function, $Z = \int D\{f^{\dagger} f\} D\{c^{\dagger} c\} D\{\chi_b\} D\{b_{\boldsymbol{r}}\} D\{a_0\} e^{-S}$ with, for $U \to \infty$

$$S = \int_0^{\beta} d\tau \quad \left\{ \frac{2}{J_h} \sum_b |\chi_b(\tau)|^2 + \frac{2}{J_k} \sum_{\boldsymbol{r}} |b_{\boldsymbol{r}}(\tau)|^2 + \sum_{\boldsymbol{i},\boldsymbol{j}} \boldsymbol{c}^{\dagger}_{\boldsymbol{i}}(\tau) \left[\partial_\tau \delta_{\boldsymbol{i},\boldsymbol{j}} - T_{\boldsymbol{i},\boldsymbol{j}} \right] \boldsymbol{c}_{\boldsymbol{j}}(\tau) \right.$$

$$+ \sum_{\boldsymbol{r}} |b_{\boldsymbol{r}}(\tau)| \left[e^{i\varphi_{\boldsymbol{r}}(\tau)} \boldsymbol{f}^{\dagger}_{\boldsymbol{r}}(\tau) \boldsymbol{c}_{\boldsymbol{r}}(\tau) + h.c. \right]$$

$$+ \sum_{\boldsymbol{r}} \boldsymbol{f}^{\dagger}_{\boldsymbol{r}}(\tau) \left[\partial_\tau - i a_{0,\boldsymbol{r}}(\tau) \right] \boldsymbol{f}_{\boldsymbol{r}}(\tau) + i a_{0,\boldsymbol{r}}(\tau) + \sum_{b = \langle \boldsymbol{r}, \boldsymbol{r}' \rangle} |\chi_b(\tau)| \left[\boldsymbol{f}^{\dagger}_{\boldsymbol{r}}(\tau) e^{-i \int_{\boldsymbol{r}}^{\boldsymbol{r}'} \boldsymbol{a}(\boldsymbol{l},\tau) d\boldsymbol{l}} \boldsymbol{f}_{\boldsymbol{r}'}(\tau) + h.c. \right]$$

Local moments in metals

$$S = \int_0^\beta d\tau \quad \Big\{ \frac{2}{J_h} \sum_b |\chi_b(\tau)|^2 + \frac{2}{J_k} \sum_{\boldsymbol{r}} |b_{\boldsymbol{r}}(\tau)|^2 + \sum_{\boldsymbol{i},\boldsymbol{j}} \boldsymbol{c}^\dagger_{\boldsymbol{i}}(\tau) \left[\partial_\tau \delta_{\boldsymbol{i},\boldsymbol{j}} - T_{\boldsymbol{i},\boldsymbol{j}} \right] \boldsymbol{c}_{\boldsymbol{j}}(\tau)$$

$$+ \sum_{\boldsymbol{r}} |b_{\boldsymbol{r}}(\tau)| \left[e^{i\varphi_{\boldsymbol{r}}(\tau)} \boldsymbol{f}^\dagger_{\boldsymbol{r}}(\tau) \boldsymbol{c}_{\boldsymbol{r}}(\tau) + h.c. \right]$$

$$+ \sum_{\boldsymbol{r}} \boldsymbol{f}^\dagger_{\boldsymbol{r}}(\tau) \left[\partial_\tau - i a_{0,\boldsymbol{r}}(\tau) \right] \boldsymbol{f}_{\boldsymbol{r}}(\tau) + i a_{0,\boldsymbol{r}}(\tau) + \sum_{b=\langle \boldsymbol{r},\boldsymbol{r}' \rangle} |\chi_b(\tau)| \left[\boldsymbol{f}^\dagger_{\boldsymbol{r}}(\tau) e^{-i \int_{\boldsymbol{r}}^{\boldsymbol{r}'} \boldsymbol{a}(\boldsymbol{l},\tau) d\boldsymbol{l}} \boldsymbol{f}_{\boldsymbol{r}'}(\tau) + h.c. \right]$$

Local U(1) gauge invariance:

$$\boldsymbol{f}^\dagger_{\boldsymbol{r}}(\tau) \rightarrow \boldsymbol{f}^\dagger_{\boldsymbol{r}}(\tau) e^{i\eta_{\boldsymbol{r}}(\tau)}$$

$$\boldsymbol{c}^\dagger_{\boldsymbol{r}}(\tau) \rightarrow \boldsymbol{c}^\dagger_{\boldsymbol{r}}(\tau)$$

$$\begin{bmatrix} a_{0,\boldsymbol{r}}(\tau) & \rightarrow a_{0,\boldsymbol{r}}(\tau) - \partial_\tau \eta_{\boldsymbol{r}}(\tau) \\ \boldsymbol{a}_{\boldsymbol{r}}(\tau) & \rightarrow \boldsymbol{a}_{\boldsymbol{r}}(\tau) - \boldsymbol{\nabla}_{\boldsymbol{r}} \eta_{\boldsymbol{r}}(\tau) \\ \varphi_{\boldsymbol{r}}(\tau) & \rightarrow \varphi_{\boldsymbol{r}}(\tau) - \eta_{\boldsymbol{r}}(\tau) \end{bmatrix}$$

Other symmetry allowed terms, such as U(1) flux, and dynamics of the b-field, will be dynamically generated.

Saeed Saremi and Patrick A. Lee, Phys. Rev. B 75 (2007), 165110.

Local moments in metals

$$S = \int_0^\beta d\tau \left\{ \frac{2}{J_h}\sum_b |\chi_b(\tau)|^2 + \frac{2}{J_k}\sum_{\boldsymbol{r}} |b_{\boldsymbol{r}}(\tau)|^2 + \sum_{\boldsymbol{i},\boldsymbol{j}} \boldsymbol{c}^\dagger_{\boldsymbol{i}}(\tau)\left[\partial_\tau \delta_{\boldsymbol{i},\boldsymbol{j}} - T_{\boldsymbol{i},\boldsymbol{j}}\right]\boldsymbol{c}_{\boldsymbol{j}}(\tau) \right.$$

$$+ \sum_{\boldsymbol{r}} |b_{\boldsymbol{r}}(\tau)| \left[e^{i\varphi_{\boldsymbol{r}}(\tau)} \boldsymbol{f}^\dagger_{\boldsymbol{r}}(\tau)\boldsymbol{c}_{\boldsymbol{r}}(\tau) + h.c.\right]$$

$$+ \sum_{\boldsymbol{r}} \boldsymbol{f}^\dagger_{\boldsymbol{r}}(\tau)\left[\partial_\tau - i a_{0,\boldsymbol{r}}(\tau)\right]\boldsymbol{f}_{\boldsymbol{r}}(\tau) + i a_{0,\boldsymbol{r}}(\tau) + \sum_{b=\langle \boldsymbol{r},\boldsymbol{r}'\rangle} |\chi_b(\tau)| \left[\boldsymbol{f}^\dagger_{\boldsymbol{r}}(\tau) e^{-i\int_{\boldsymbol{r}}^{\boldsymbol{r}'} \boldsymbol{a}(\boldsymbol{l},\tau)d\boldsymbol{l}} \boldsymbol{f}_{\boldsymbol{r}'}(\tau) + h.c.\right]$$

Classification of Phases	$\langle \boldsymbol{f}^\dagger_{\boldsymbol{r}}\boldsymbol{\sigma}\boldsymbol{f}_{\boldsymbol{r}}\rangle \neq 0$	$\langle b_{\boldsymbol{r}}\rangle \neq 0$ $e^{i\varphi} f^\dagger = \tilde{f}^\dagger$	Gauge field
Kondo	✗	✓	confined
SDW	✓	✗	confined
Kondo + SDW	✓	✓	confined
FL*	✗	✗	De-confined
SDW*	✓	✗	De-confined

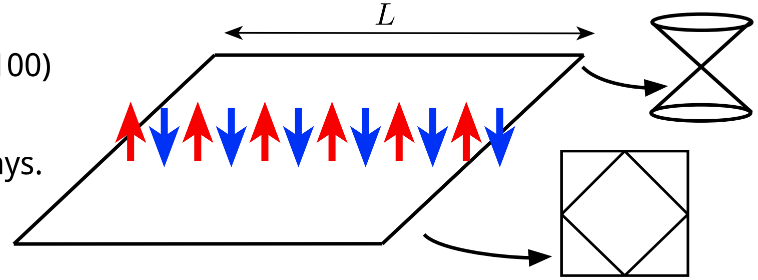
Julius-Maximilians-
UNIVERSITÄT
WÜRZBURG

Local moments in metals

Toy models to realize **metallic** phases and phase transitions in Kondo systems (FL*, FL, LRO) without confronting the sign problem.

Co atoms on $Cu_2N/Cu(100)$

R. Toskovic et al. Nat. Phys. 2016



Kondo breakdown transitions and phases

B. Danu, M. Vojta, FFA, and T. Grover, Phys. Rev. Lett. 125 (2020), 206602.

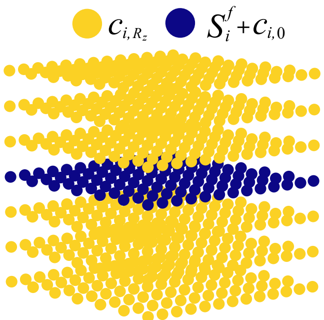
Dissipation induced magnetic order-disorder transitions

B. Danu, M. Vojta, T. Grover FFA, Phys. Rev. B 106 (2022), L161103.

M. Weber, D. J. Luitz, and FFA, Phys. Rev. Lett. 129 (2022), 056402.

$LaIn_3/CeIn_3$

H. Shishido et al. Science 2010



Marginal Fermi liquid at magnetic quantum criticality from dimensional confinement

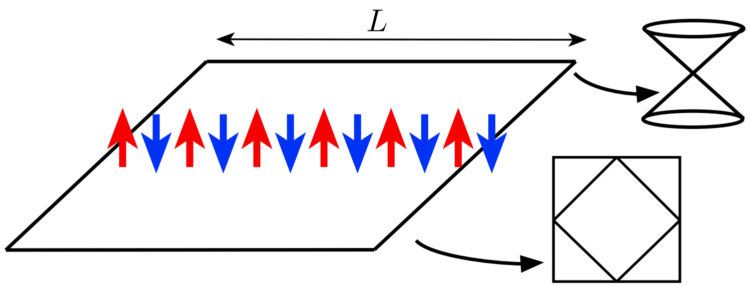
Zi Hong Liu, B. Frank, L. Janssen, M. Vojta, FFA, Phys. Rev. B 107, 165104 (2023)

B. Frank, Zi Hong Liu, FFA, M. Vojta, and L. Janssen, Phys. Rev. B 108 (2023), L100405.

$$\hat{H} = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} (\hat{\boldsymbol{c}}_{\boldsymbol{i}}^{\dagger} \hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) + \frac{J_k}{2} \sum_{\boldsymbol{r}} \hat{\boldsymbol{c}}_{\boldsymbol{r}}^{\dagger} \boldsymbol{\sigma} \hat{\boldsymbol{c}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}} + J_h \sum_{\langle \boldsymbol{r},\boldsymbol{r}' \rangle} \hat{\boldsymbol{S}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}'}$$

Local moments in metals

Kondo phase @ $J_k/t >> 1$

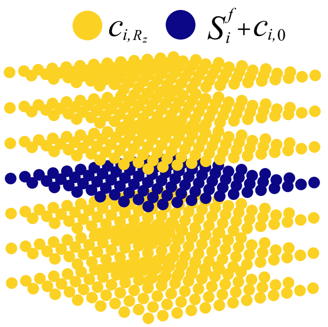


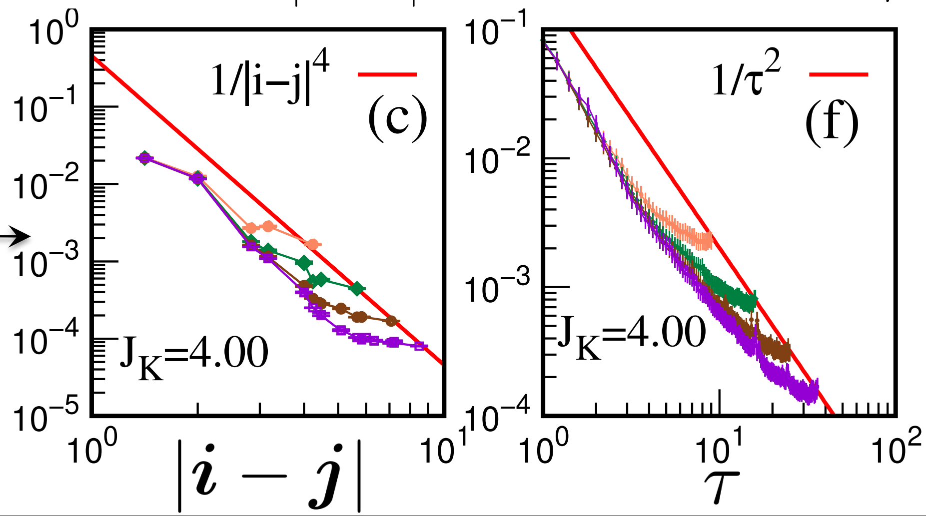
$$\hat{H} = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} (\hat{\boldsymbol{c}}^{\dagger}_{\boldsymbol{i}} \hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) + \frac{J_k}{2} \sum_{\boldsymbol{r}} \hat{\boldsymbol{c}}^{\dagger}_{\boldsymbol{r}} \boldsymbol{\sigma} \hat{\boldsymbol{c}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}} + J_h \sum_{\langle \boldsymbol{r},\boldsymbol{r}' \rangle} \hat{\boldsymbol{S}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}'}$$

$e^{i\varphi} f^{\dagger} = \tilde{f}^{\dagger}$ Emergent composite fermion that participates in Luttinger count

Spin-spin correlations inherit power-law of conduction electrons.

$$\langle \hat{\boldsymbol{S}}_{\boldsymbol{r}} \hat{\boldsymbol{S}}_{\boldsymbol{r}'} \rangle \propto \frac{1}{|\boldsymbol{r} - \boldsymbol{r}'|^4} \qquad \langle \hat{\boldsymbol{S}}_{\boldsymbol{r}}(\tau) \hat{\boldsymbol{S}}_{\boldsymbol{r}}(0) \rangle \propto \frac{1}{\tau^2}$$

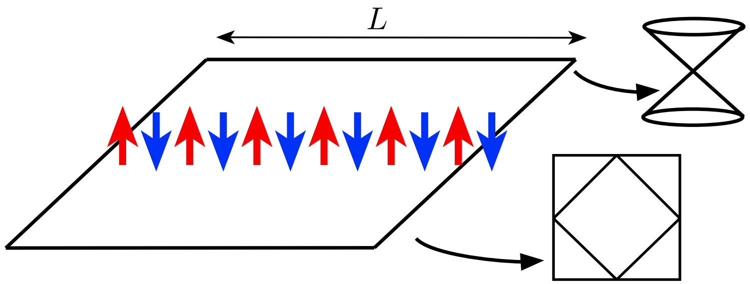




$$\langle \boldsymbol{f}^{\dagger}_{\boldsymbol{i}}(\tau) \boldsymbol{\sigma} \boldsymbol{f}_{\boldsymbol{i}}(\tau) \cdot \boldsymbol{f}^{\dagger}_{\boldsymbol{j}}(0) \boldsymbol{\sigma} \boldsymbol{f}_{\boldsymbol{j}}(0) \rangle = \langle \tilde{\boldsymbol{f}}^{\dagger}_{\boldsymbol{i}}(\tau) \boldsymbol{\sigma} \tilde{\boldsymbol{f}}_{\boldsymbol{i}}(\tau) \cdot \tilde{\boldsymbol{f}}^{\dagger}_{\boldsymbol{j}}(0) \boldsymbol{\sigma} \tilde{\boldsymbol{f}}_{\boldsymbol{j}}(0) \rangle$$

Spin chain on semi-metal

B. Danu, M. Vojta, FFA, and T. Grover, Phys. Rev. Lett. 125 (2020), 206602.

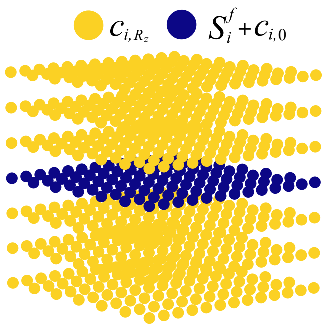


$$\hat{H} = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} (\hat{\boldsymbol{c}}^{\dagger}_{\boldsymbol{i}} \hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) + \frac{J_k}{2} \sum_{\boldsymbol{r}} \hat{\boldsymbol{c}}^{\dagger}_{\boldsymbol{r}} \boldsymbol{\sigma} \hat{\boldsymbol{c}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}} + J_h \sum_{\langle \boldsymbol{r},\boldsymbol{r}' \rangle} \hat{\boldsymbol{S}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}'}$$

Integrate out electrons à la Hertz-Millis

$$\mathcal{S}(\boldsymbol{n}) = \mathcal{S}_{\text{spin}}(\boldsymbol{n}) + \mathcal{S}_{\text{diss}}(\boldsymbol{n}) + \cdots$$

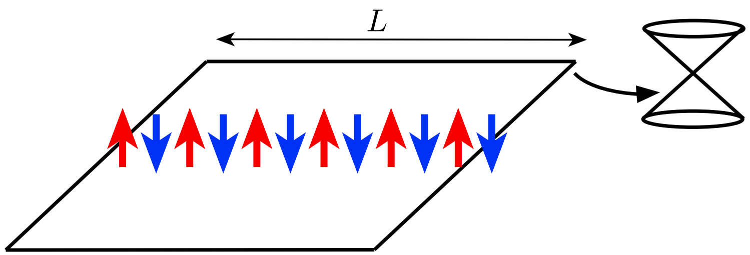
$$\mathcal{S}_{\text{diss}}(\boldsymbol{n}) = \frac{J_k^2}{8} \int d\tau d\tau' \sum_{\boldsymbol{r},\boldsymbol{r}'} \boldsymbol{n}_{\boldsymbol{r}}(\tau) \chi^0(\boldsymbol{r} - \boldsymbol{r}', \tau - \tau') \boldsymbol{n}_{\boldsymbol{r}'}(\tau').$$



Spin susceptibility of the host metal

Spin chain on semi-metal

B. Danu, M. Vojta, FFA, and T. Grover, Phys. Rev. Lett. 125 (2020), 206602.



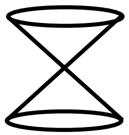
$$\hat{H} = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} (\hat{\boldsymbol{c}}^\dagger_{\boldsymbol{i}} \hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) + \frac{J_k}{2} \sum_{\boldsymbol{r}} \hat{\boldsymbol{c}}^\dagger_{\boldsymbol{r}} \boldsymbol{\sigma} \hat{\boldsymbol{c}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}} + J_h \sum_{\langle \boldsymbol{r},\boldsymbol{r}' \rangle} \hat{\boldsymbol{S}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}'}$$

Integrate out electrons à la Hertz-Millis

$$\mathcal{S}(\boldsymbol{n}) = \mathcal{S}_{\text{spin}}(\boldsymbol{n}) + \mathcal{S}_{\text{diss}}(\boldsymbol{n}) + \cdots$$

$$\mathcal{S}_{\text{diss}}(\boldsymbol{n}) = \frac{J_k^2}{8} \int d\tau d\tau' \sum_{\boldsymbol{r},\boldsymbol{r}'} \boldsymbol{n}_{\boldsymbol{r}}(\tau) \chi^0(\boldsymbol{r}-\boldsymbol{r}', \tau-\tau') \boldsymbol{n}_{\boldsymbol{r}'}(\tau').$$

$$\Delta_n = \frac{1}{2}$$



$$\chi^0(\boldsymbol{0}, \tau-\tau') \propto \frac{1}{v_F^2 (\tau-\tau')^4}$$

$$\chi^0(r\boldsymbol{e}_x, 0) \propto \frac{1}{r^4}$$

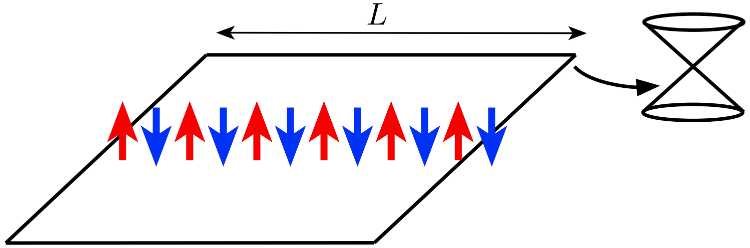
Kondo is irrelevant

For: $\boldsymbol{r} \to \lambda \boldsymbol{r}, \ \tau \to \lambda \tau$,

$$\mathcal{S}_{\text{diss}}(\boldsymbol{n}) = \frac{J_k^2}{8} \int d\tau d\tau' d\boldsymbol{r}\, \boldsymbol{n}_{\boldsymbol{r}}(\tau) \chi^0(0, \tau-\tau') \boldsymbol{n}_{\boldsymbol{r}}(\tau') \to \lambda^{-2} \mathcal{S}_{\text{diss}}(\boldsymbol{n})$$

Spin chain on semi-metal

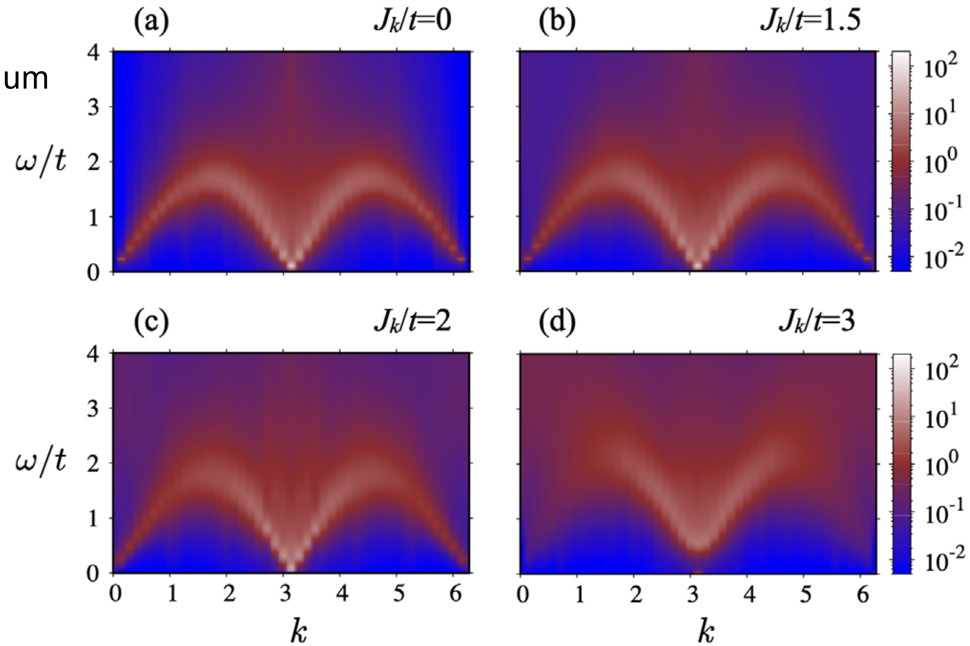
B. Danu, M. Vojta, FFA, and T. Grover, Phys. Rev. Lett. 125 (2020), 206602.



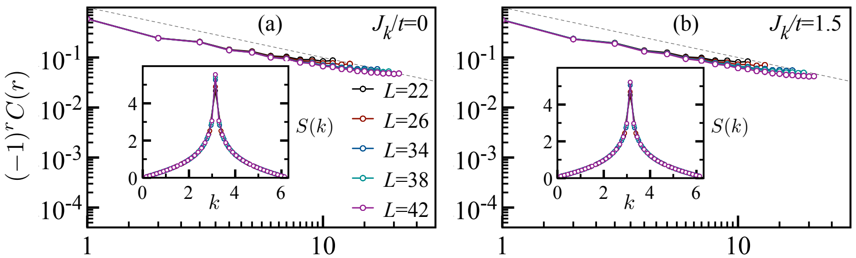
$$\hat{H} = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} (\hat{\boldsymbol{c}}^{\dagger}_{\boldsymbol{i}} \hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) + \frac{J_k}{2} \sum_{\boldsymbol{r}} \hat{\boldsymbol{c}}^{\dagger}_{\boldsymbol{r}} \boldsymbol{\sigma} \hat{\boldsymbol{c}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}} + J_h \sum_{\langle \boldsymbol{r},\boldsymbol{r}' \rangle} \hat{\boldsymbol{S}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}'}$$

$$S(\boldsymbol{q},\omega) = \frac{\chi''(\boldsymbol{q},\omega)}{1 - e^{-\beta\omega}}$$

Two spinon continuum



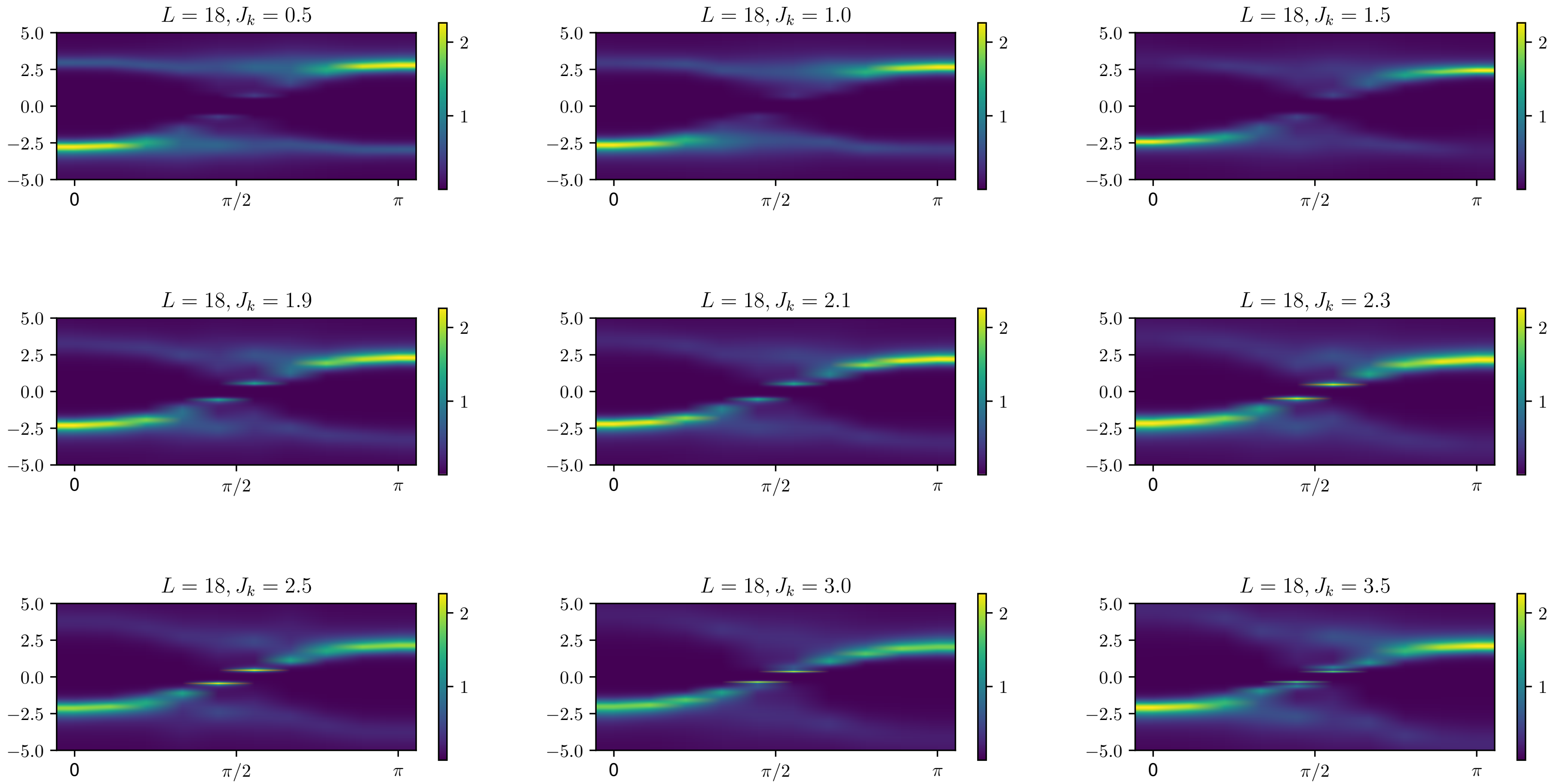
$S(\boldsymbol{q})$



Spin chain on semi-metal

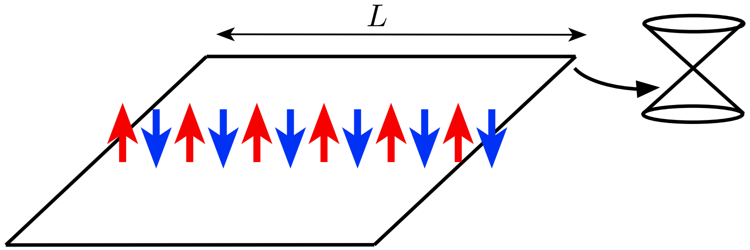
B. Danu, M. Vojta, FFA, and T. Grover, Phys. Rev. Lett. 125 (2020), 206602.

$e^{i\varphi} f^\dagger = \tilde{f}^\dagger$ Composite fermion spectral function



Spin chain on semi-metal

B. Danu, M. Vojta, FFA, and T. Grover, Phys. Rev. Lett. 125 (2020), 206602.



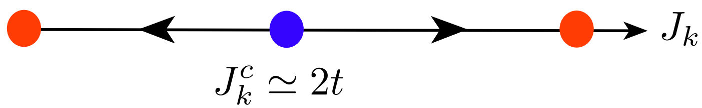
$$\hat{H} = -t\sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle}(\hat{\boldsymbol{c}}^{\dagger}_{\boldsymbol{i}}\hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) + \frac{J_k}{2}\sum_{\boldsymbol{r}}\hat{\boldsymbol{c}}^{\dagger}_{\boldsymbol{r}}\boldsymbol{\sigma}\hat{\boldsymbol{c}}_{\boldsymbol{r}}\cdot\hat{\boldsymbol{S}}_{\boldsymbol{r}} + J_h\sum_{\langle \boldsymbol{r},\boldsymbol{r}'\rangle}\hat{\boldsymbol{S}}_{\boldsymbol{r}}\cdot\hat{\boldsymbol{S}}_{\boldsymbol{r}'}$$

FL*

$\langle b\rangle = 0,\ \langle \boldsymbol{n}\rangle = 0$

Heavy fermion metal

$\langle b\rangle \neq 0,\ \langle \boldsymbol{n}\rangle = 0$

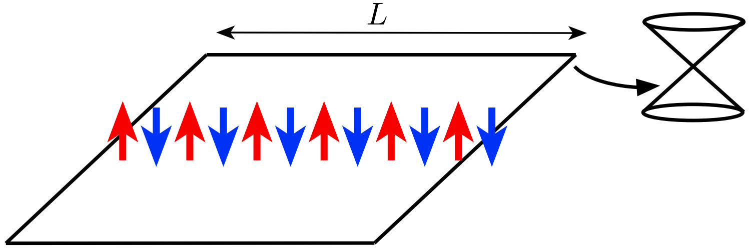


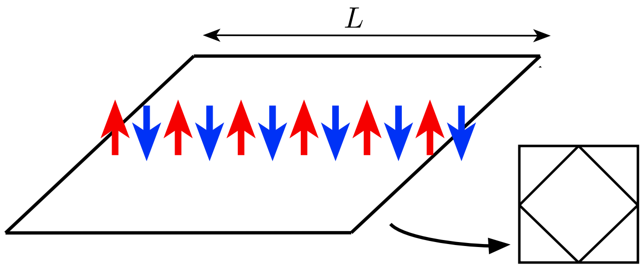
Questions:

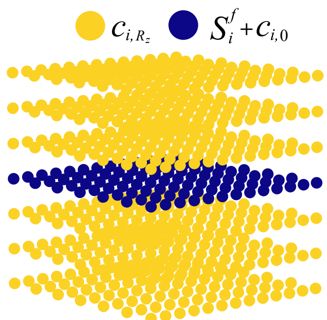
1) Critical exponents ?
2) Transport ?
3) Unique realization of Kondo Breakdown transition → playground to investigate various entanglement measures and witnesses. F. Mazza et al. arXiv:2403.12779.

Local moments in metals

Summary II







Dimensional mismatch Kondo systems

$$\hat{H} = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} (\hat{\boldsymbol{c}}_{\boldsymbol{i}}^{\dagger} \hat{\boldsymbol{c}}_{\boldsymbol{j}} + h.c) + \frac{J_k}{2} \sum_{\boldsymbol{r}} \hat{\boldsymbol{c}}_{\boldsymbol{r}}^{\dagger} \boldsymbol{\sigma} \hat{\boldsymbol{c}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}} + J_h \sum_{\langle \boldsymbol{r},\boldsymbol{r}' \rangle} \hat{\boldsymbol{S}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{r}'}$$

Magnetic impurities are sub-intensive

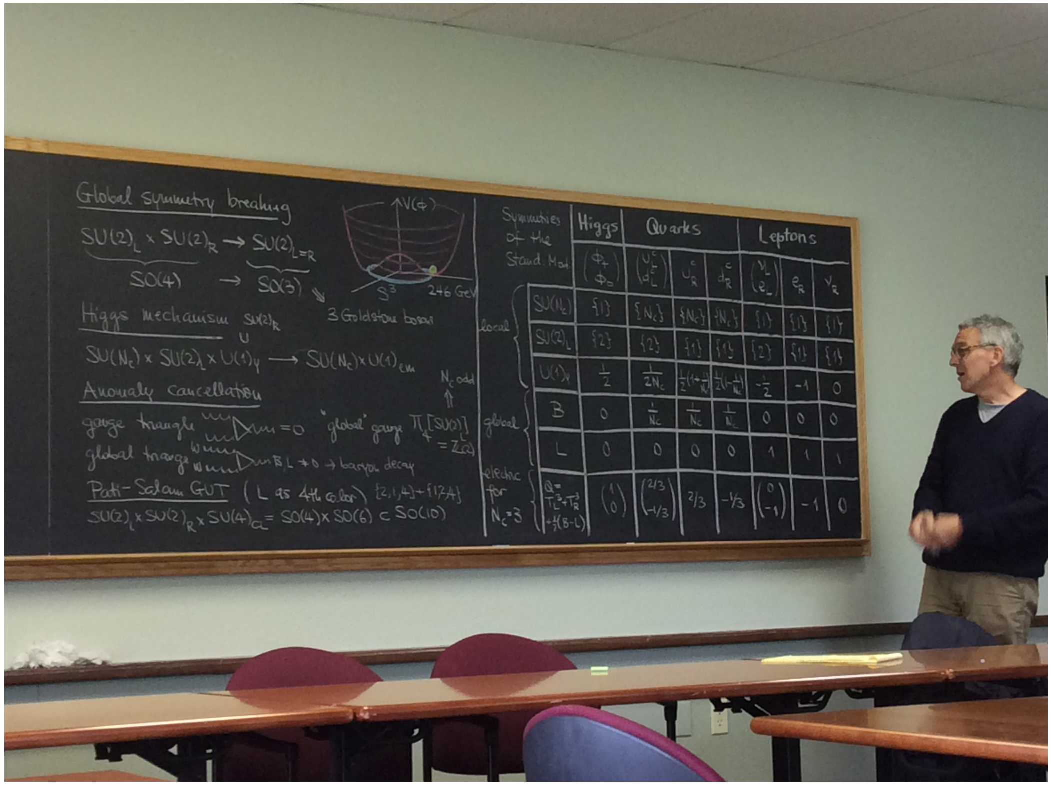
No nesting instability even at particle-hole symmetry

Negative sign free models that realize metallic phases of heavy fermion systems. Experimentally relevant.

Confronting the sign problem for frustrated magnets

Fakher F. Assaad, Workshop on the sign problem in QCD and beyond, Bern, January 20-24, 2025

Aspen, June, 2015



Thank you for promoting interdisciplinary research !