Functional renormalization group as an approach to frustrated magnetism

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Santa Barbara, September 24, 2019

Motivation

We apply the functional renormalization group (FRG) method to spin models of the form

$$H = \sum_{ij} J_{ij}\, \vec{S}_i \vec{S}_j$$

- on 2D and 3D lattices (with sites labeled i, j)
- frustrated and longer-range interactions J_{ij} possible
- anisotropic interactions $J_{ij}^{xx} \neq J_{ij}^{yy} \neq J_{ij}^{zz}$, $J_{ij}^{xy} \neq 0$, etc. possible (*)
- spin magnitudes $S = 1/2,\ 1,\ 3/2,\ \ldots$

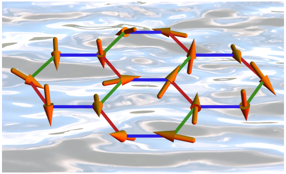
$\Longrightarrow$ **Pseudofermion functional renormalization group (PFFRG)**

*terms and conditions apply (but relatively few)

Motivation

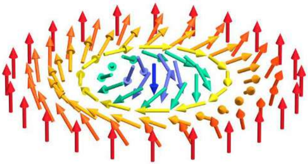
Why magnetic spin systems?

- Exotic quantum phases



spin liquid

- Interesting spin textures

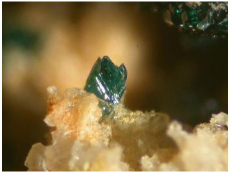


skyrmion

- Topological properties

fractional quasiparticles

- Material realizations



Herbertsmithite ($ZnCu_3(OH)_6Cl_2$)

Outline

Pseudo fermions

Pseudo fermions

Introduce two fermionic operators $f_{i\uparrow}$, $f_{i\downarrow}$ for each lattice site i. Rewrite:

$$S_i^\mu = \frac{1}{2}\sum_{\alpha,\beta} f_{i,\alpha}^\dagger \sigma_{\alpha\beta}^\mu f_{i,\beta}$$

with $\{f_{i\alpha}, f_{i\beta}^\dagger\} = \delta_{\alpha\beta}$ and $\sigma^\mu =$ Pauli matrices

Enlarged Hilbert space

Basis set $|n_{i\uparrow}, n_{i\downarrow}\rangle$ for one lattice site i:

$|0,0\rangle$ $|0,1\rangle$ $|1,0\rangle$ $|1,1\rangle$

$|\downarrow\rangle$ $|\uparrow\rangle$

$\Longrightarrow$ pseudo fermions come along with an enlarged Hilbert space.

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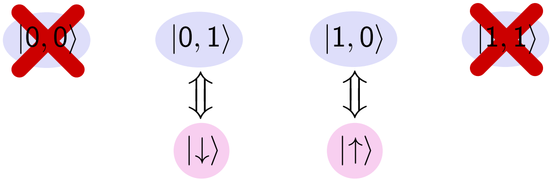

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Constraint $f^\dagger_{i\uparrow} f_{i\uparrow} + f^\dagger_{i\downarrow} f_{i\downarrow} = 1$ needs to be fulfilled!

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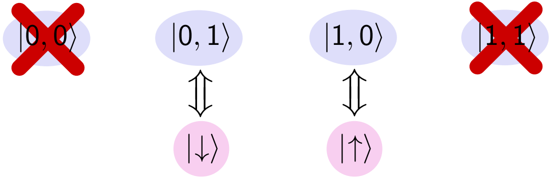

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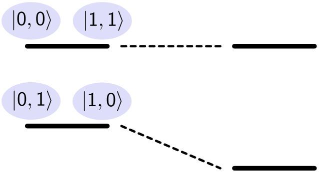
Constraint $f^\dagger_{i\uparrow} f_{i\uparrow} + f^\dagger_{i\downarrow} f_{i\downarrow} = 1$ needs to be fulfilled!

Convenient way to enforce the constraint:
Level repulsion terms:

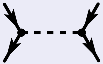
$$H \to H - A\sum_i (\mathbf{S}_i)^2 = H - A\sum_i S_i(S_i+1)$$



Fermionic Hamiltonian

$$H = \sum_{ij} J_{ij}\, \vec{S}_i \vec{S}_j \longrightarrow \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \sum_{ij} J_{ij} \left(f^{\dagger}_{i,\alpha} \sigma^{\mu}_{\alpha\beta} f_{i\beta} \right) \left(f^{\dagger}_{j,\gamma} \sigma^{\mu}_{\gamma\delta} f_{j,\delta} \right)$$

Diagrammatics in the fermions:

progagator: $G_0(i\omega) = \frac{1}{i\omega} =$    interaction vertex: $\Gamma_0 =$  $\sim J$

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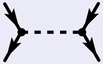
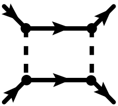
progagator: $G_0(i\omega) = \frac{1}{i\omega} =$    interaction vertex: $\Gamma_0 =$  $\sim J$

Magnetic susceptibility, spin-spin correlations:



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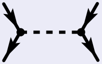
progagator: $G_0(i\omega) = \frac{1}{i\omega} =$    interaction vertex: $\Gamma_0 =$  $\sim J$

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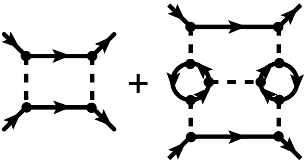

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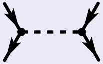
progagator: $G_0(i\omega) = \frac{1}{i\omega} =$    interaction vertex: $\Gamma_0 =$  $\sim J$

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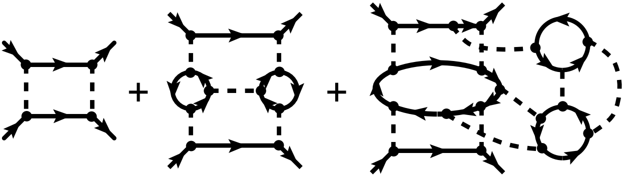


Fermionic Hamiltonian

Since there is no small parameter, self-consistent infinite order diagrammatic summations need to be performed:

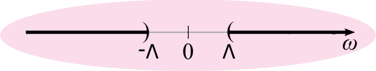
Functional renormalization group (FRG)

Functional renormalization group

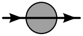
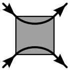
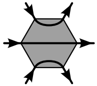
Functional renormalization group

Introduce infrared frequency cutoff in the propagator:

$G_0(i\omega) = \frac{1}{i\omega} \quad \longrightarrow \quad G_0^\Lambda(i\omega) = \frac{\Theta(|\omega|-\Lambda)}{i\omega}$

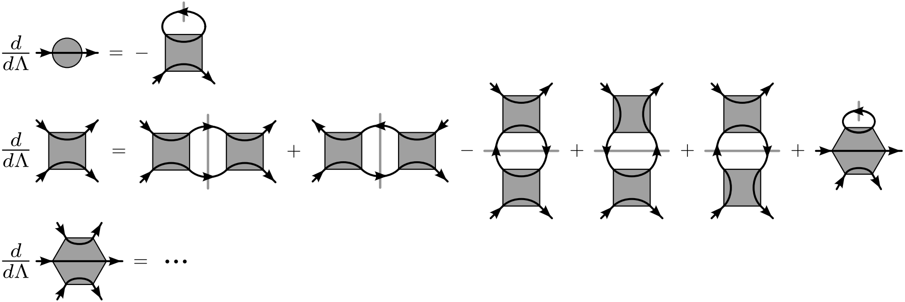


Then all vertex functions become Λ-dependent:

$\Sigma =$  $\longrightarrow \quad \Sigma^\Lambda\,, \quad \Gamma =$  $\longrightarrow \quad \Gamma^\Lambda\,, \quad \Gamma_3 =$  $\longrightarrow \quad \Gamma_3^\Lambda$

Functional renormalization group

FRG formulates flow equations for all *m*-particle vertex functions:



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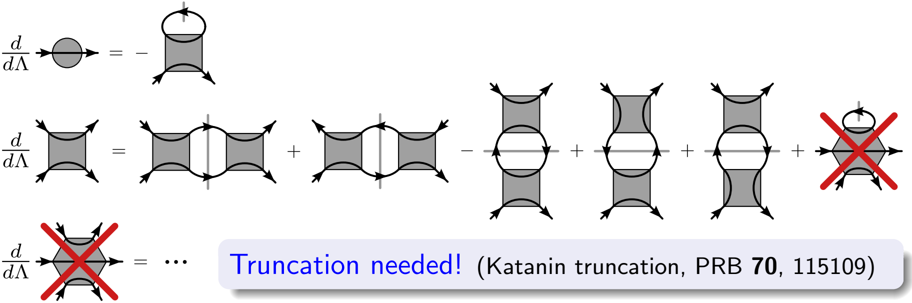

Truncation needed! (Katanin truncation, PRB **70**, 115109)

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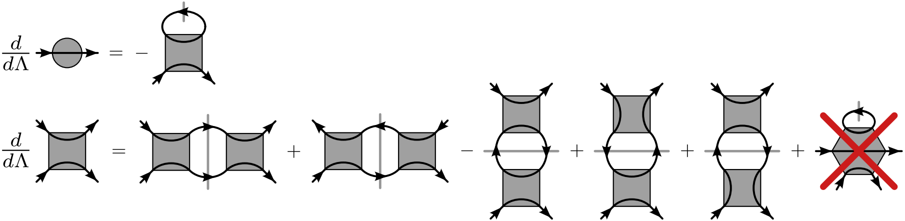
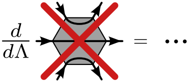
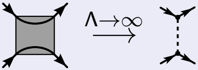
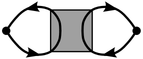




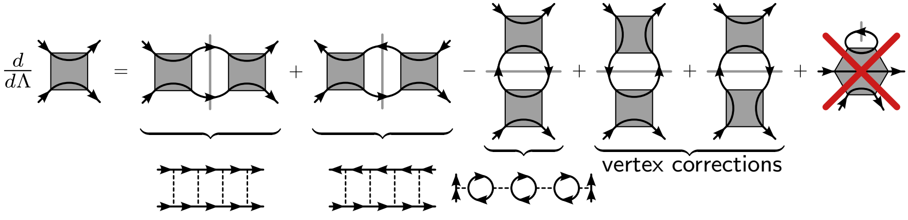
Truncation needed! (Katanin truncation, PRB **70**, 115109)

Flow starts with  $\sim J$ and ends at $\Lambda = 0$.

Calculate magnetic susceptibility $\frac{\partial M}{\partial B}$: $\chi^{\Lambda}(\mathbf{k}) =$ 

Functional renormalization group

FRG sums up diagrammatic contributions in infinite order in J.



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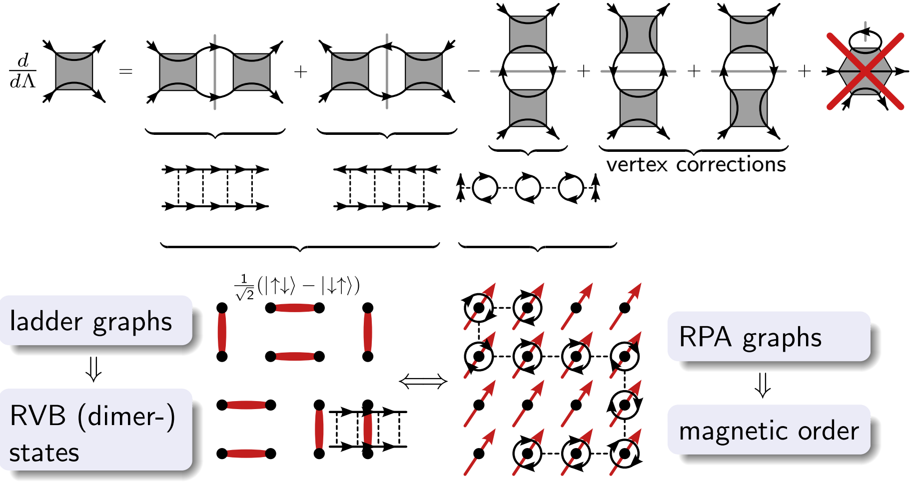

Functional renormalization group

Here: spin-$\frac{1}{2}$, $SU(2)$ representation

Generalization: spin-S, $SU(N)$ representation

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Order and disorder tendencies are equally included in the one-loop FRG

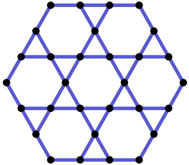
FRG equations are solved in real space with the full frequency dependence of the vertex functions. System sizes of $\sim$2000 lattice sites are possible.

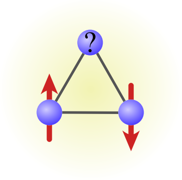
Applications and benchmarks: 2D kagome lattice

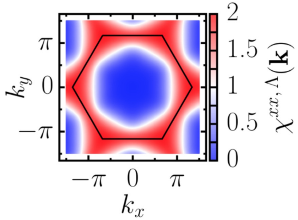
Kagome antiferromagnet

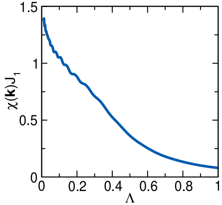
$$H = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \mathbf{S}_j \; , \quad J_1 > 0$$

temperature $T = 0$









non-magnetic ground state!

R. Suttner, JR, et al., PRB **89**, 020408 (2014)

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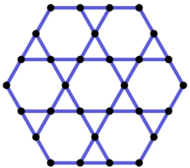

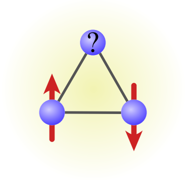

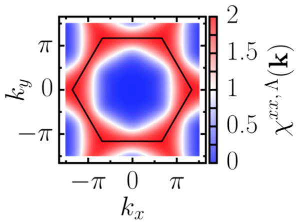

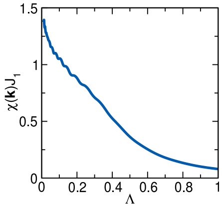

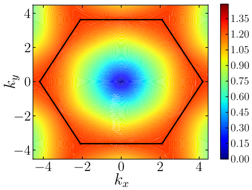

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Comparison: DMRG

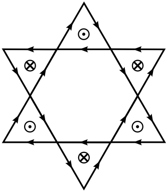
S. Depenbrock et al.,

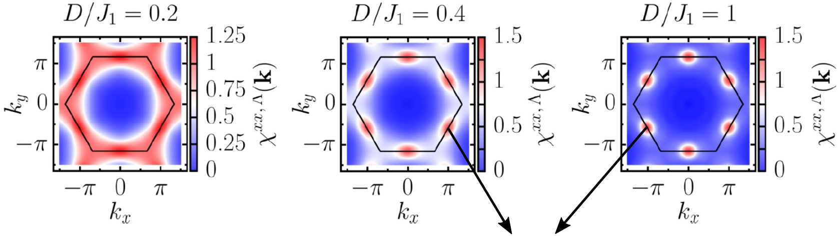
PRL **109**, 067201 (2012)

Kagome antiferromagnet

Include Dzyaloshinskii-Moriya interactions:

$$H = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \mathbf{S}_j + \sum_{\langle ij \rangle} D_{ij} (\mathbf{S}_i \times \mathbf{S}_j)_z$$





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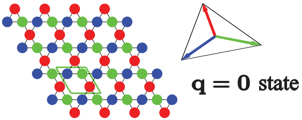
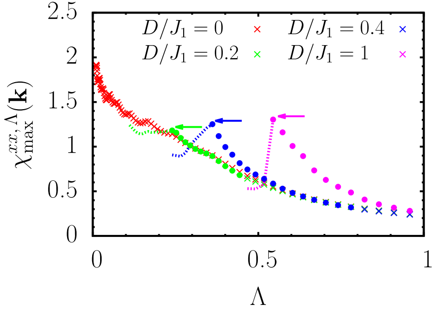


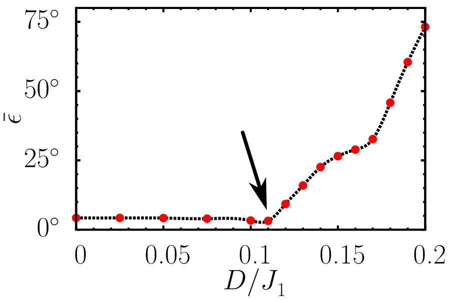
PRB 95, 054418

Kagome antiferromagnet

RG flow:



Instability feature:



Phase transition at $D/J_1 = 0.11 \ldots 0.12$

Comparison with ED: $D/J_1 \approx 0.1$ (O. Cepas, et al., PRB **78**, 140405(R) (2008))

$Ca_{10}Cr_7O_{28}$

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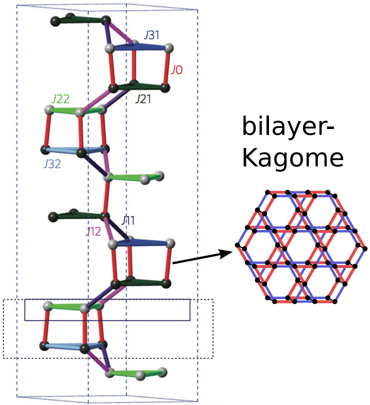
$Ca_{10}Cr_7O_{28}$ consists of stacked spin-1/2 bilayer Kagome planes:



C. Balz, B. Lake, JR et al.,

Nature Physics (2016)

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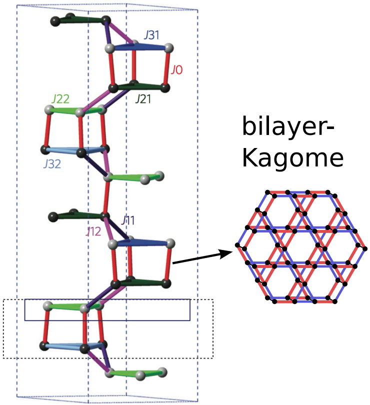

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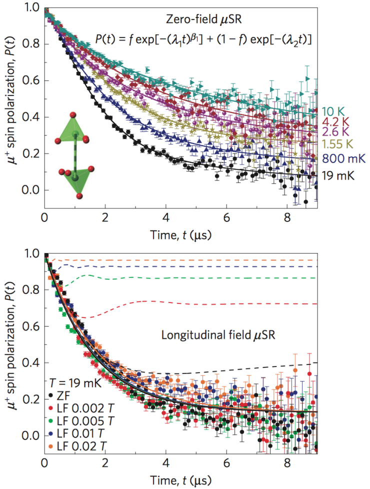
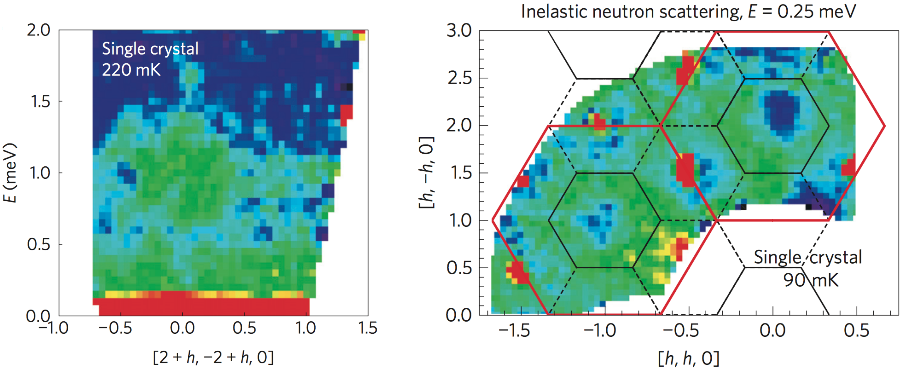
Moun spin relaxation measurements rule out static magnetic order down to 19mK:



$Ca_{10}Cr_7O_{28}$

Insights from inelastic neutron scattering:

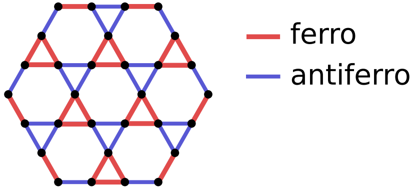


Inelastic neutron scattering finds very broad (spinon-like) spin excitations with ring-shaped features in momentum space.

$Ca_{10}Cr_7O_{28}$

Determination of exchange couplings J: Spin waves have been measured by neutron scattering in a magnetic field and fitted to spin wave theory.

Result: Each Kagome layer consists of ferromagnetic and antiferromagnetic nearest neighbor couplings.



Top layer:
$J_{\mathrm{FM}} = -0.27 meV$, $J_{AF} = 0.09 meV$
Bottom layer:
$J_{\mathrm{FM}} = -0.76 meV$, $J_{AF} = 0.11 meV$

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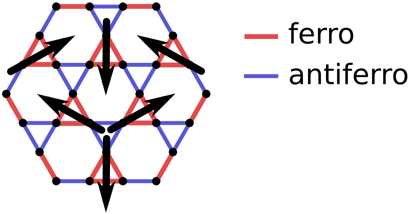

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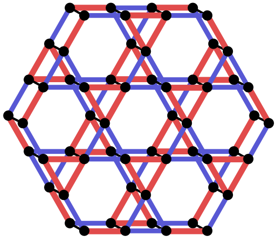
$\Longrightarrow$ effective spin-$3/2$ system would form 120°-Néel order!?

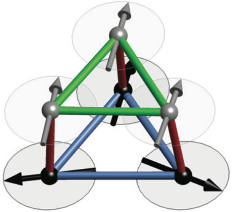
$Ca_{10}Cr_7O_{28}$

Where does the frustration come from?



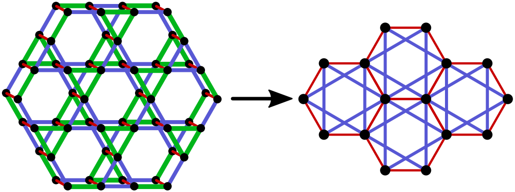
- FM triangles lie on top of AF triangles
- FM coupling of $J_\perp = -0.08 meV$ between the layers

$\Longrightarrow$ Very strong frustration mechanism!



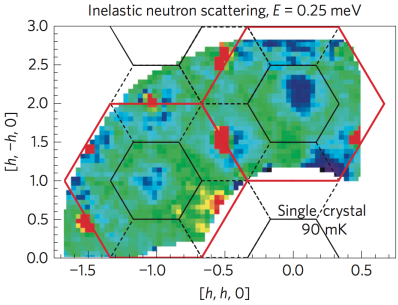
$Ca_{10}Cr_7O_{28}$: Previous theory works

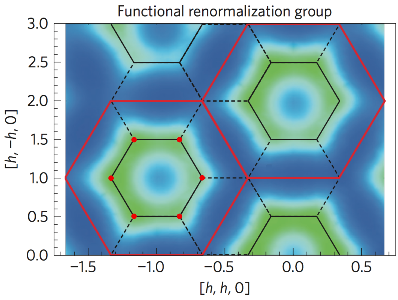
- C. Balz, B. Lake, JR et al., Nature Physics **12**, 942 (2016)
  Experiment + theory (functional renormalization)
- R. Pohle, H. Yan, and N. Shannon, arXiv:1711.03778
  MD simulations, spin-3/2 honeycomb mapping



- S. Biswas and K. Damle, Phys. Rev. B **97**, 115102 (2018)
  Semiclassical analysis, spin-3/2 honeycomb mapping
- A. Kshetrimayum, C. Balz, B. Lake, and J. Eisert, arXiv:1904.00028
  Tensor network approach

$Ca_{10}Cr_7O_{28}$

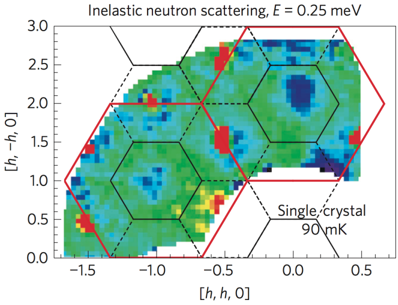


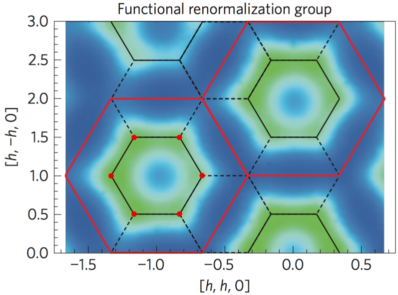


Comparison of neutron scattering versus FRG:

120°-Néel order is destroyed, yielding broad rings in momentum space.

$Ca_{10}Cr_7O_{28}$

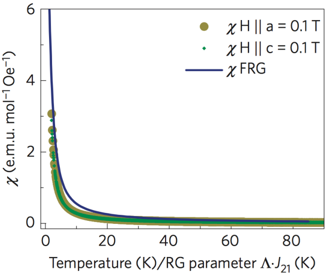




Comparison of neutron scattering versus FRG:

120°-Néel order is destroyed, yielding broad rings in momentum space.

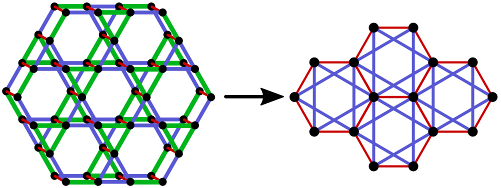
Flowing FRG-susceptibility is smooth showing no indication of a magnetic instability:

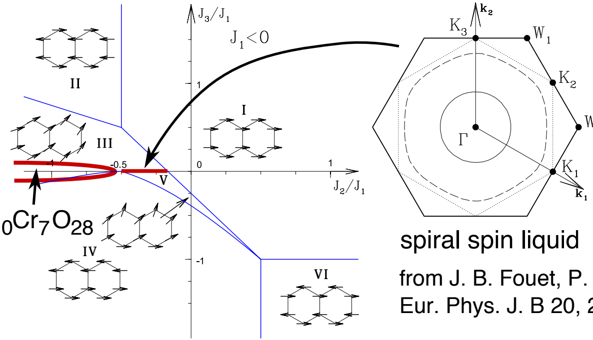


Origin of ring-like response

Mapping onto spin-3/2 honeycomb Heisenberg model with FM J_1 and AFM J_2

$J_2/J_1 \approx -3.1, \ldots, -0.6$





spiral spin liquid

from J. B. Fouet, P. Sindzingre, and C. Lhuillier, Eur. Phys. J. B 20, 241 (2001)

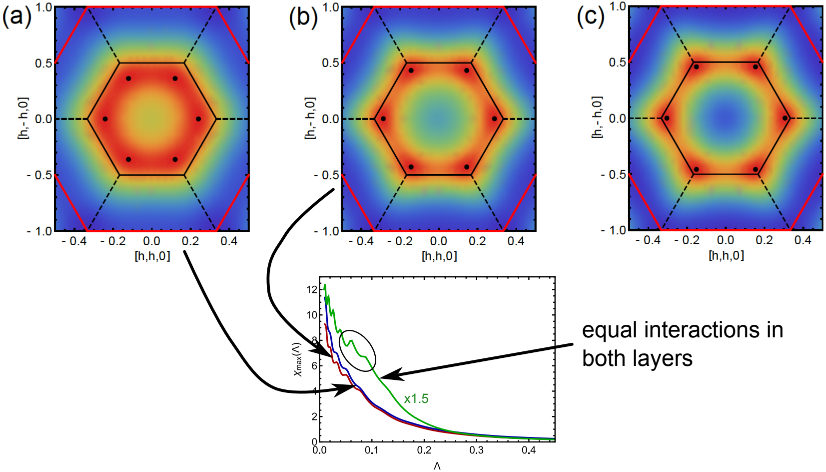
R. Pohle, H. Yan, and N. Shannon, arXiv:1711.03778

Varying the exchange couplings

AFM intralayer couplings are rescaled by 1/2

unchanged

FM intralayer couplings are rescaled by 1/2

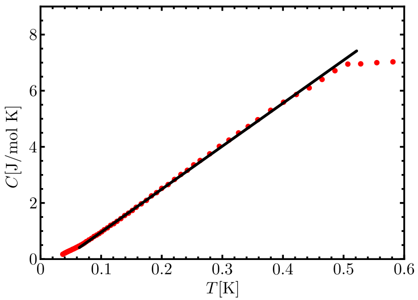


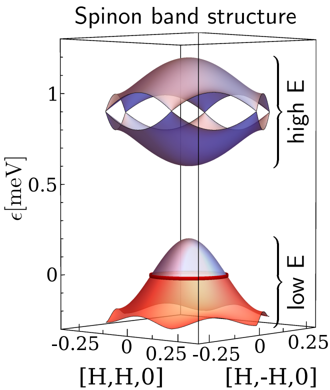
Remarkable stability of the SL phase, asymmetric interactions important!

Extensions/Outlook

Extensions/Outlook

- Possible nature of spin liquid in $Ca_{10}Cr_7O_{28}$?
  Almost perfect linear heat capacity below 0.5 K!
  Spinon Fermi surface?





J. Sonnenschein, C. Balz, B. Lake, JR et al. arXiv:1905.06761 (2019)

Determine spinon bands directly from PFFRG:

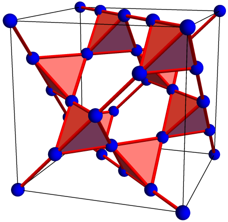
M. Hering, J. Sonnenschein, Y. Iqbal, and JR, Phys. Rev. B 99, 100405(R) (2019)

Extensions/Outlook

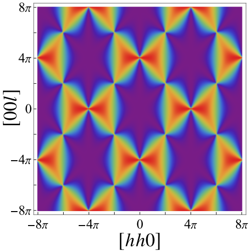
- 3D systems: Example: nn pyrochlore Heisenberg antiferromagnet

$H = J_1 \sum_{ij} \vec{S}_i \vec{S}_j$ (Y. Iqbal, JR, H. O. Jeschke, et al., PRX 9, 011005 (2019))

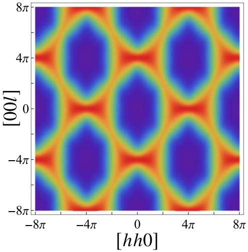
pyrochlore lattice



$S \to \infty$

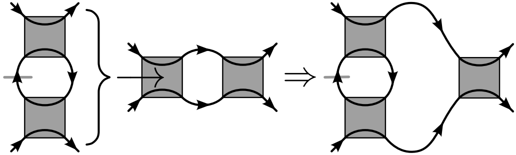


$S = 1/2$



Extensions/Outlook

- higher-loop PFFRG:
  Two-loop already implemented (M. Rück and JR, PRB 97, 144404 (2018)).



Extensions/Outlook

- higher-loop PFFRG:
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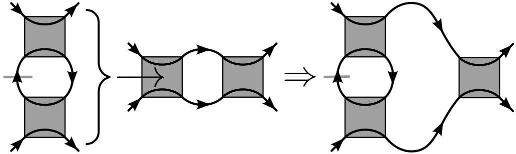
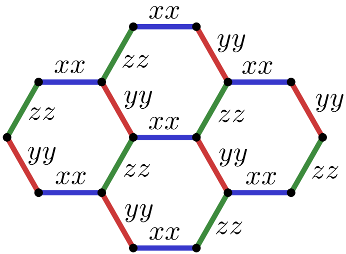


- Majorana PFFRG ($\longrightarrow$ Kitaev models, in progress)



Conclusion

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- ✓ PFFRG allows to investigate a large class of spin systems (Heisenberg, Dzyaloshinskii-Moriya,Γ, Kitaev, XXZ, long-range J).
- ✓ 2D and 3D lattices.
- ✓ Large systems with $\sim$ 2000 sites.
- ✓ Higher spins $S > 1/2$ possible.

Conclusion

- ✔ PFFRG allows to investigate a large class of spin systems (Heisenberg, Dzyaloshinskii-Moriya,Γ, Kitaev, XXZ, long-range J).
- ✔ 2D and 3D lattices.
- ✔ Large systems with $\sim$ 2000 sites.
- ✔ Higher spins $S > 1/2$ possible.

- ✘ Couplings beyond two-body interactions cannot be treated.
- ✘ No dynamic response functions (yet).
- ✘ 1D systems are not accessible.
- ✘ Critical regions are hard to explore.

Collaborators

Theory:

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V. Noculak (Berlin)

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M. Nissen (Berlin)

CRC183 ENTANGLED STATES OF MATTER

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Y. Iqbal (Chennai)

R. Thomale (Würzburg)

H. O. Jeschke (Okayama)

B. Sbirski (Berkeley)

S. Rachel (Melbourne)

M. Gingras (Waterloo)

Experiment:

B. Lake (Berlin)

S. Chillal (Berlin)

S. Nagler (Oakridge)

C. Balz (Oakridge)

Thank you for your attention!