Pseudo Majorana Functional Renormalisation Group for Quantum Spin Systems

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Freie Universität Berlin, Helmholtz Zentrum Berlin

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The group

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Freie Universität Berlin   HZB Helmholtz Zentrum Berlin   CRC183 ENTANGLED STATES OF MATTER

Introduction

(Spin liquids and their excitations)

Ordered states of matter

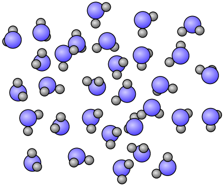
Usually, matter "freezes" at sufficiently low temperatures
$\Longrightarrow$ it form a more ordered state

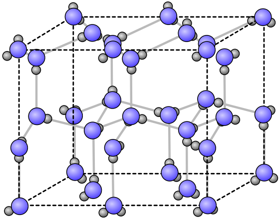
Examples:

T<0°C

water

ice





disordered liquid

regular crystal

pictures: pixabay.com

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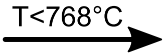
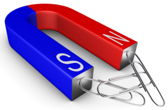
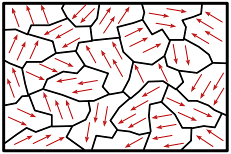


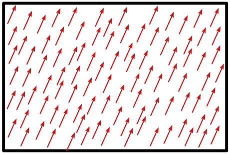


iron, paramagnetic

iron, ferromagnetic



many domains



single domain

pictures: pixabay.com

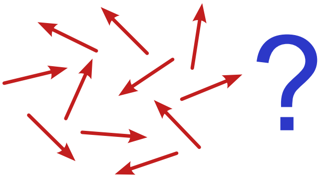
Spin liquids

Our research interest:

Magnetic states of matter and materials which remain liquid (disordered, dynamic) down to $T = 0K$.

Spin liquids

$\Longrightarrow$ Special mechanism to keep the spins disordered are needed.



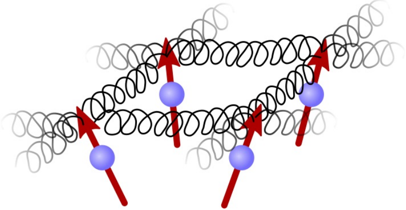
Basics: Microscopic situation

Consider interacting electron spins (spin-1/2) on a lattice.

Simplest (and most realistic) type of interaction:

Heisenberg couplings (spin isotropic)

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

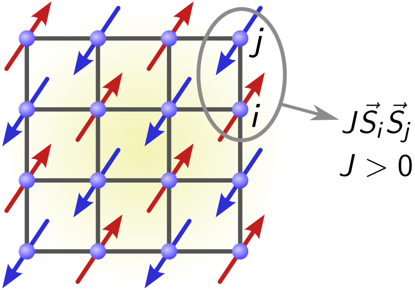


Basics: Antiferromagnetic interactions

Heisenberg couplings naturally arise in insulating materials with strong electron interactions (Mott insulator).

$\Longrightarrow$ Electrons cannot move $\Longrightarrow$ spin degree of freedom important!

$\Longrightarrow$ Interactions are antiferromagnetic, i.e. spins want to align antiparallel.



Simplest case:

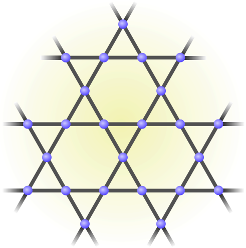
Spin-1/2 Heisenberg antiferromagnet on square lattice

$$H = \sum_{\langle ij \rangle} J\vec{S}_i\vec{S}_j$$

Magnetic order: Néel state

Magnetic frustration

What happens for antiferromagnetic triangles? (e.g. Kagome lattice)



Magnetic frustration

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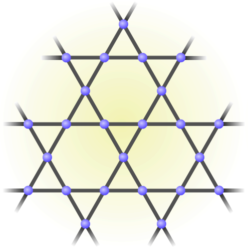

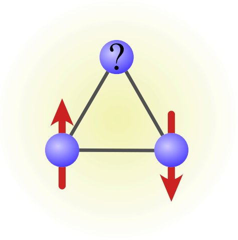

$\Longrightarrow$ **Magnetic frustration**

Terms in H cannot all be simultaneously minimized!

Magnetic frustration

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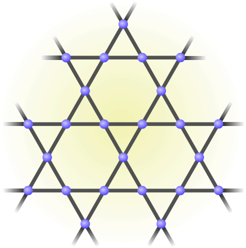
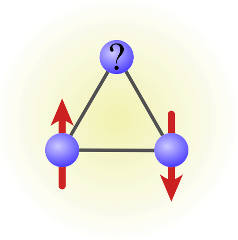




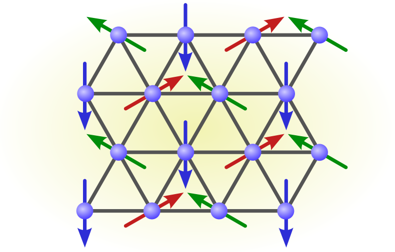
$\Longrightarrow$ **Magnetic frustration**

Terms in H cannot all be simultaneously minimized!

Possibility 1:

Spins find a compromise.

Example:
120° Néel order on triangular lattice.

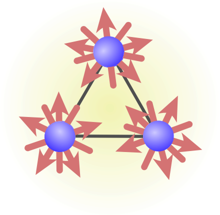


Many other interesting types of orders exist (e.g. spin spirals).

Magnetic frustration

Possibility 2:

Use properties from quantum mechanics:
Spin don't have to point in any specific direction. The directions can fluctuate.



$\Longrightarrow$ **Novel spin state:**

Quantum spin liquid

No magnetic order: $\langle \Psi | \vec{S}_i | \Psi \rangle = 0$

Quantum mechanical description?

Spin singlets

Simplest spin state with $\langle\Psi|\vec{S}_i|\Psi\rangle = 0$?

Two spins in a singlet $|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle\right)$

Is also ground state of $H = J\vec{S}_1\vec{S}_2$ for $J > 0$

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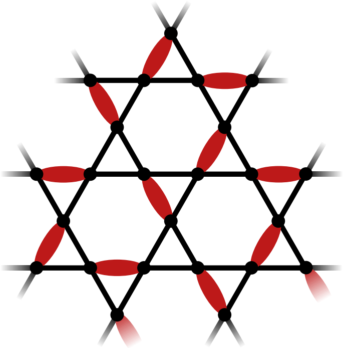
Pair up spins on the lattice into singlet bonds:

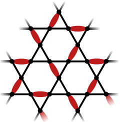
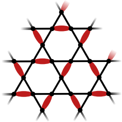
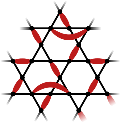


Non-magnetic state

But still static!

Resonating valence bond state

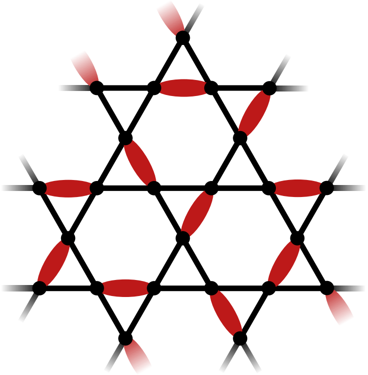
Solution: Superimpose macroscopically many singlet configurations!

$|\Psi\rangle = a_1|$  $\rangle + a_2|$  $\rangle + a_3|$  $\rangle + \ldots$

= resonating valence bond (RVB) state. (Anderson, Baskaran, 1987)

Magnetic excitations: Spinons

Break up a singlet dimer into two aligned spins (= spin-1 excitation):



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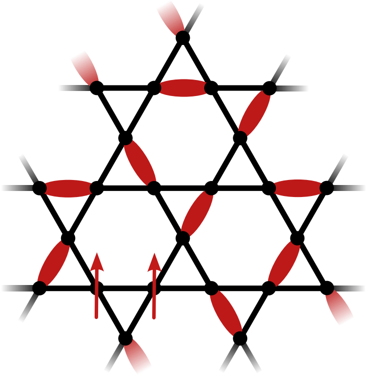

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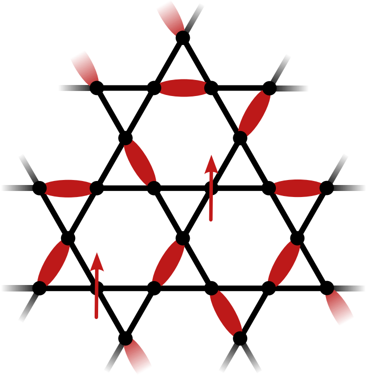

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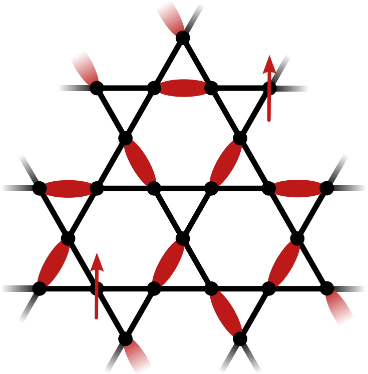


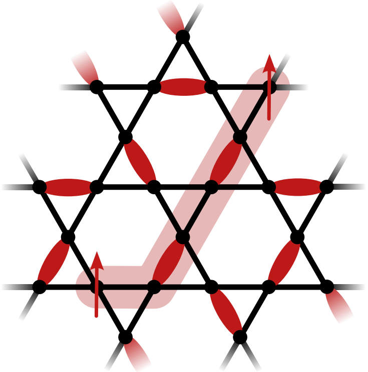
Isolated spins are effectively free (deconfined).

$\Longrightarrow$ New quasiparticles: spinons. Carry spin $\frac{1}{2}$!

Fractional excitations

Rearranged dimer background

Fractional spinons are connected by a string of rearranged dimers:



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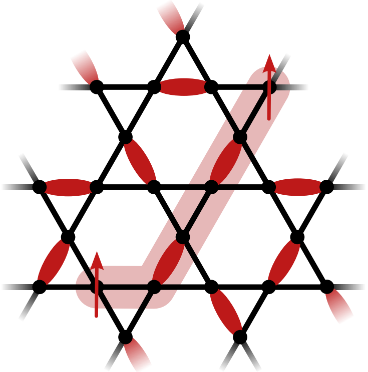
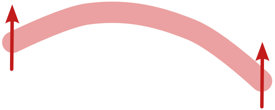
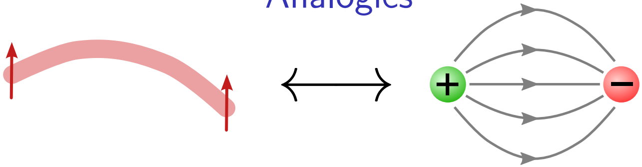


Basic ingredients for a spin liquid at low energies:



- Spinons.
- Strings connecting them.

Analogies



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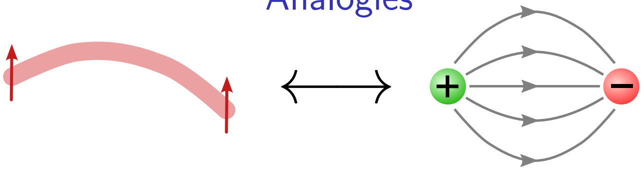
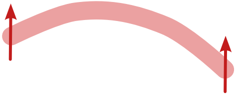


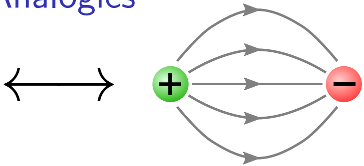
Spinons ⟷ Charged particles
(“matter fields”, e.g. electrons)

Strings ⟷ Field lines
(“gauge fields”, e.g. electric field)

Spin liquid ⟷ Theories from fundamental physics

Analogies





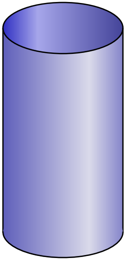
Spinons	⟷	Charged particles
		(“matter fields”, e.g. electrons)
Strings	⟷	Field lines
		(“gauge fields”, e.g. electric field)
Spin liquid	⟷	**Theories from fundamental physics**

A spin liquid realizes theories otherwise only known from fundamental physics → playground for finding new physics in exotic states of matter.

- Emergent electrodynamics (spin ice materials).
- Majorana fermions (half electrons) in Kitaev spin liquids.
- Effective gravity in spin-1 magnets.

Topological properties of spin liquids

Fractional excitations and topological ground state degeneracy:



spin liquid in ground-state $|1\rangle$

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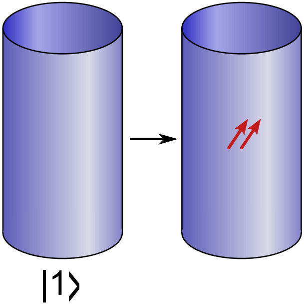

spin liquid in ground-state $|1\rangle$

$\longrightarrow$ create pair of spinons

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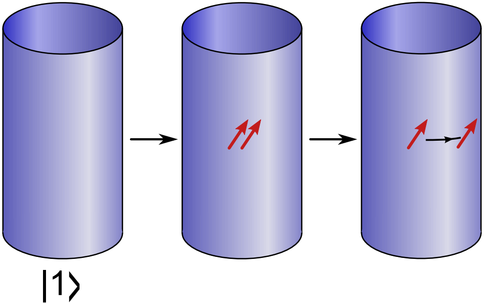

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$\longrightarrow$ create pair of spinons

$\longrightarrow$ wind one spinon around cylinder

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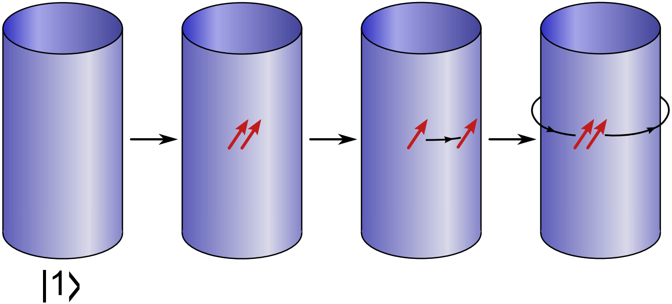

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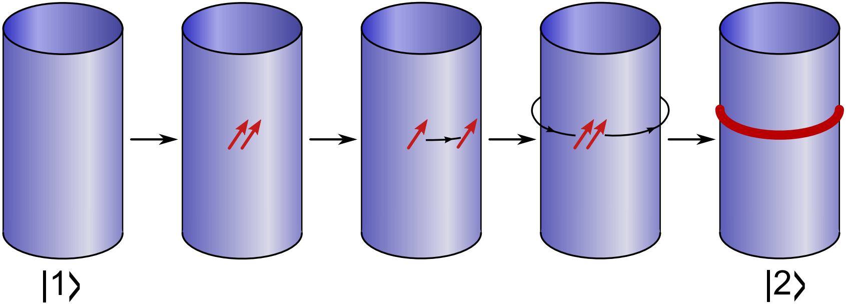


spin liquid in ground-state $|1\rangle$

$\longrightarrow$ create pair of spinons

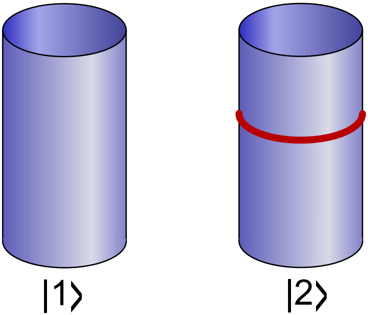
$\longrightarrow$ wind one spinon around cylinder

$\longrightarrow$ annihilate spinons, end up in ground state $|2\rangle \neq |1\rangle$

Possible quantum information applications

Transition from $|1\rangle$ to $|2\rangle$ requires non-local operation.

$\longrightarrow$ **quantum information is topologically protected!**



Idea: Use the states $|1\rangle$ and $|2\rangle$ as stable qubit states.

Quantum spin liquids in experiments

Spinons can only be created in pairs!

Do spin-1 excitation with energy E and momentum q:

$\longrightarrow$ Decomposition into spinon 1 with energy ϵ_1 and momentum k_1
and spinon 2 with energy ϵ_2 and momentum k_2.

$\longrightarrow$ Continuum of possibilities such that $E = \epsilon_1 + \epsilon_2$ and $q = k_1 + k_2$

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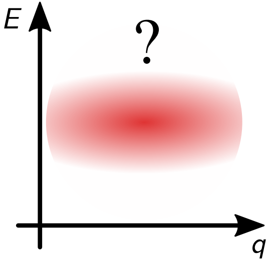
Excitation spectrum:

Quantum spin liquid



two-spinon continuum

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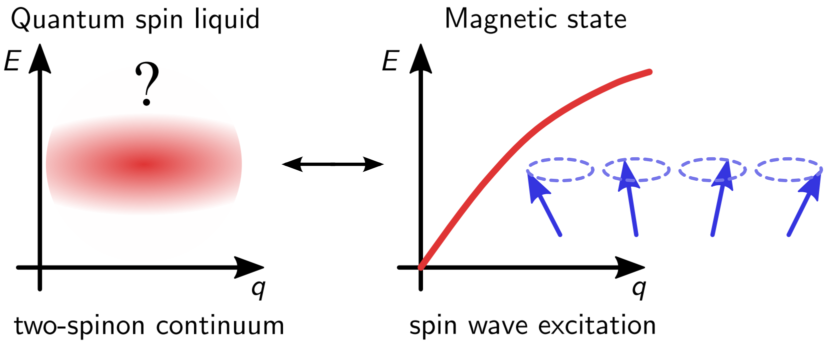

Numerical methods: PFFRG and PMFRG

Review article: T. Müller, D. Kiese, N. Niggemann, B. Sbierski, JR, S. Trebst, R. Thomale, and Y. Iqbal, *Pseudo-fermion functional renormalization group for spin models*, Rep. Prog. Phys. 87, 036501 (2024)

Pseudo fermions

Starting point: $H = \sum_{ij} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$

Express spin operators in terms of pseudo fermions: $\boldsymbol{S} = \frac{1}{2} \sum_{\alpha\beta \in \uparrow,\downarrow} f_\alpha^\dagger \boldsymbol{\sigma}_{\alpha\beta} f_\beta$
where $\{f_\alpha, f_\beta^\dagger\} = \delta_{\alpha\beta}$.

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Be careful: Enlarged Hilbert space with unphysical non- and doubly occupied states.

Experience: Unphysical states are excitations. Application at $T = 0$.

Exceptions: B. Schneider, D. Kiese, and B. Sbierski, PRB 106, 235113 (2022)

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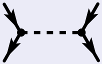
$$H = \sum_{ij} J_{ij}\, \boldsymbol{S}_i \cdot \boldsymbol{S}_j \longrightarrow \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \sum_{ij} J_{ij} \left(f_{i\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} f_{i\beta} \right) \cdot \left(f_{j\gamma}^\dagger \boldsymbol{\sigma}_{\gamma\delta} f_{j\delta} \right)$$

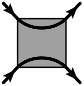
Diagrammatics in the fermions:

Progagator: $G_0(i\omega) = \frac{1}{i\omega} =$ 

Interaction vertex: $\Gamma_0 =$  $\sim J$

Functional renormalization group

Magnetic susceptibility, spin-spin correlations, spin structure factor:



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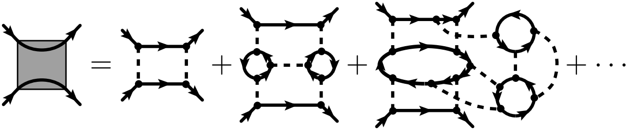

Sampling problem for Feynman diagrams! Efficient resummation scheme:

Functional renormalization group (FRG)

Metzner, Salmhofer, Honerkamp, Meden, Schönhammer, RMP 84, 299 (2012)

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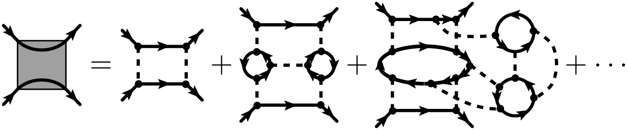

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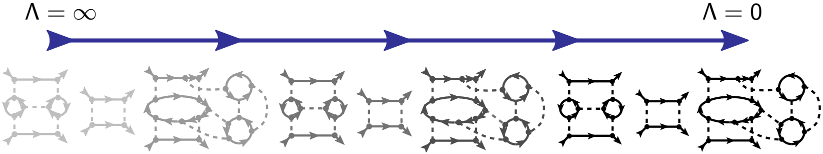
Sum up Feynman diagrams during the flow of an RG parameter Λ:



Functional renormalization group

Example: Implementation of Λ as a low frequency cutoff in $G_0(i\omega)$:

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

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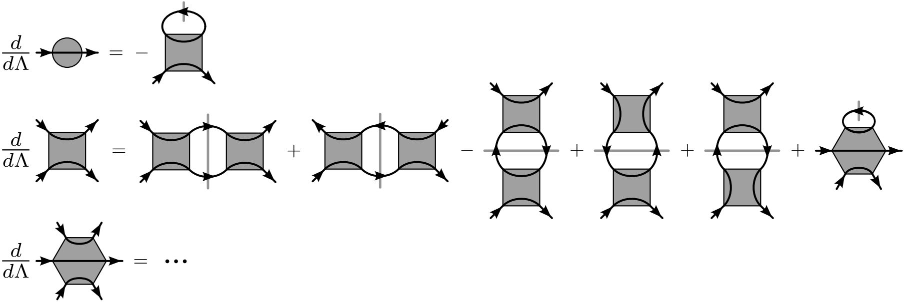

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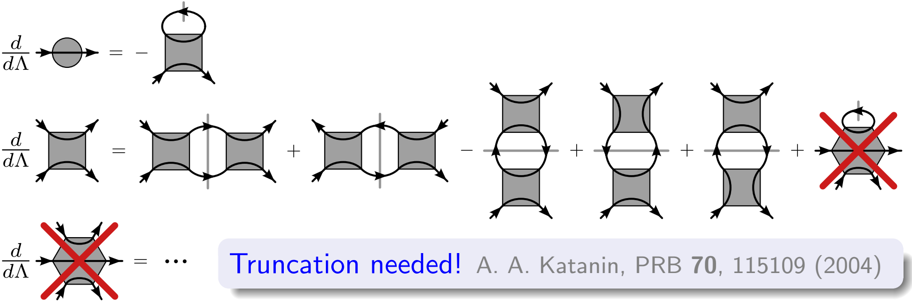
FRG formulates differential equations for all *m*-particle vertex functions:



Truncation needed! A. A. Katanin, PRB **70**, 115109 (2004)

Pseudofermion functional renormalization group (PFFRG)

J. Reuther and P. Wölfle, PRB 81, 144410 (2010)

Pseudo Majorana functional renormalization group

Alternatively: Express spin operators in terms of Majorana fermions:

$S^{\mu} = -\frac{i}{4} \sum_{\nu\sigma \in x,y,z} \epsilon_{\mu\nu\sigma} c^{\nu} c^{\sigma}$ with $(c^{\mu})^2 = 1$.

Advantage: No unphysical states, only redundant Hilbert spaces!
Applicable at $T > 0$.

Pseudo Majorana functional renormalization group (PMFRG)

N. Niggemann, B. Sbierski, and JR, PRB 103, 104431 (2021)

N. Niggemann, JR, B. Sbierski, SciPost Phys. 12, 156 (2022)

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N. Niggemann, B. Sbierski, and JR, PRB 103, 104431 (2021)

N. Niggemann, JR, B. Sbierski, SciPost Phys. 12, 156 (2022)

Higher efficiency with temperature-flow approach where $\Lambda = T$!

C. Honerkamp and M. Salmhofer, PRB 64, 184516 (2001)

Facts about the code

- Main challenge: Solving large systems of coupled ODEs but does not require much memory.
- Benefits greatly from parallelization (openMP and MPI parallelized).
- Language: Julia (older code in C++), public package: *https://github.com/NilsNiggemann/PMFRG.jl*
- $\sim$ 15 years of code development.
- Possibility to generate lattices automatically from VESTA files $\rightarrow$ easy to work with complicated models.

Application example:

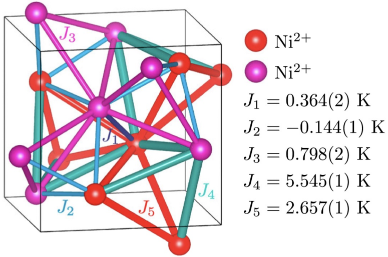
Spin liquid candidate

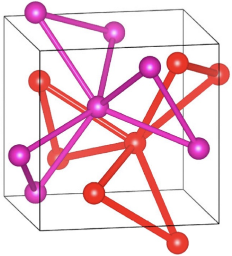
$K_2Ni_2(SO_4)_3$

M. Gonzalez, JR et al., Nature Communications 15, 7191 (2024)

Lattice structure of $K_2Ni_2(SO_4)_3$

$K_2Ni_2(SO_4)_3$ has spin-1, Ni^{2+}, two interpenetrating trillium lattices!



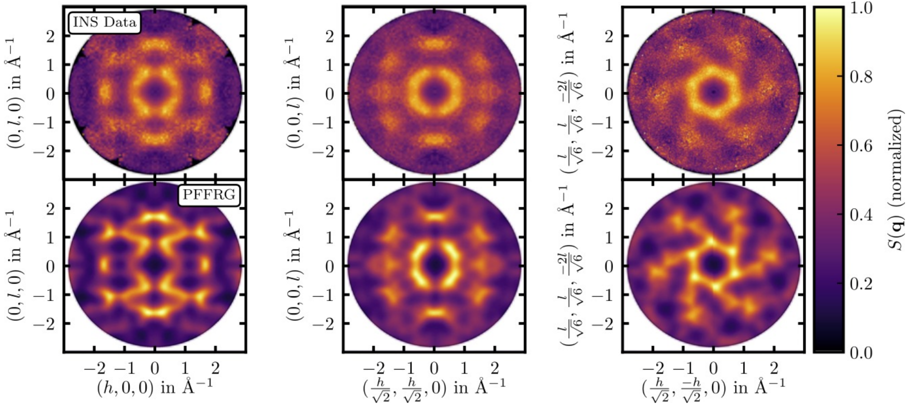


Interactions J_1, J_2, J_3, J_4, J_5 are strongest.

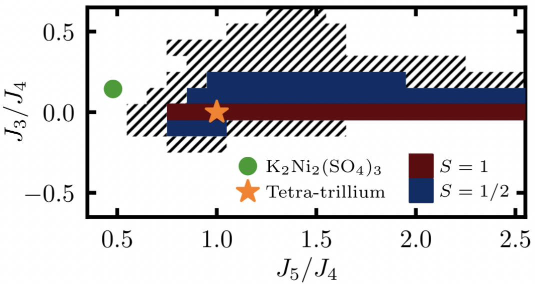
J_1, J_2, J_4: Inter-trillium couplings, J_4 largest
J_3, J_5: Intra-trillium couplings

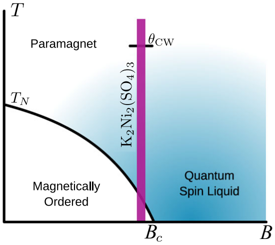
$K_2Ni_2(SO_4)_3$: Theory versus experiment

Spin structure factor $\mathcal{S}(\boldsymbol{q})$ from PFFRG and from neutron scattering:



$K_2Ni_2(SO_4)_3$: Phase diagram





- Phase diagram contains 'island of liquidity' close to $K_2Ni_2(SO_4)_3$.
- Model of $K_2Ni_2(SO_4)_3$ shows weak magnetic order (also seen in experiments).
- Small modifications, e.g. by magnetic field can induce spin liquid.

Type of spin liquid? To be continued....

Conclusions

- Spin liquids are exotic states of matter realizing emergent phenomena, e.g. theories from fundamental physics.
- The models describing spin liquids and possible candidate materials are among the hardest in physics research.
- PFFRG and PMFRG are methods that are capable of dealing with these complicated models.
- The methods are ideal for simulating magnetic quantum materials, and the results are in good agreement with measurements.

Thank you for your attention!