Master project: **Functional renormalization for quantum spins: A numerical approach**

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Introduction Quantum spin systems harbor a wealth of interesting phenomena and are intensively studied both experimentally and theoretically. Active research areas include the low energy physics of frustrated systems giving rise to spin liquid ground states without magnetic order [1] or the unusual spin diffusion recently observed in spin-1/2 chains [2]. On the theory side, the challenge is to tackle the complexity of the associated spin Hamiltonians which come in an innocuous and simple forms like in the case of the paradigmatic quantum Heisenberg model,

$$H = \frac{1}{2}\sum_{i,j} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j.$$

While exact solutions are limited to a few celebrated cases like the Kitaev spin model [3], the majority of theoretical insights rest on numerical approaches mostly based on matrix-product state approximations for the wavefunction. While tremendously successful in one dimension and rapidly improving in two dimensions, their performance is poor when it comes to three spatial dimensions or long-time dynamics. In order to cope with these challenges, a complementary approach to quantum spin systems based on the functional renormalization group (fRG) has been proposed about a decade ago [4]. This approach rests on a representation of, say, spin-1/2 operators using auxiliary spinful fermions $S_i^\mu = \frac{1}{2}\sum_{\alpha,\beta=\uparrow,\downarrow} f_{i\alpha}^\dagger \sigma_{\alpha\beta}^\mu f_{i\beta}$. The resulting interacting fermionic Hamiltonian can then be treated with well-established fRG techniques [5]. For a recent technical advancement of this pseudo-fermion fRG by our group, see Ref. [6].

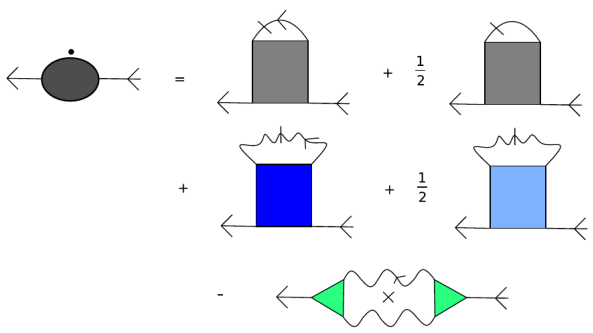
Despite certain merits of the described methods, the representation of spin operators with auxiliary fermions has serious drawbacks like the enlargement of Hilbert space and the representation of two-point spin correlators by much more complex four-point fermionic correlation functions. This prompted Peter Kopietz from Frankfurt to propose an alternative fRG approach [7] that directly works with spin correlation functions without taking a detour via auxiliary particle representations. In the last two years, the Frankfurt group has refined their method even further [8]–[10] and obtained promising results for observables like magnon damping rates or dynamic spin structure factors. However, the full potential of their formalism is still to be revealed. In order to do this, solutions to their flow equations must be computed numerically, a challenging task that however should be achievable with our group's existing expertise.

Project roadmap

- Formalism: Familiarize yourself with the basic idea of the fRG [5], [11], then understand the spin-fRG formalism developed in [7] and the follow up papers by Peter Kopietz and coworkers. The central equations can be translated in diagrammatic language as shown in the figure below. Reproduce their analytical results for the various scenarios and observables they consider.
- Establish numerical code: Set up a computer program that solves the spin-fRG flow equations for the vertex functions. As a first check, reproduce the published analytical results. Next, drop the simplifying assumptions in the benchmark problems one by one at the cost of systematic increase in numerical complexity. You will get support by your supervisors and other group members who over the years have gained significant expertise of solving similar flow equations.
- Phase diagrams of quantum magnets: As a final application, use the spin-fRG formalism for various frustrated quantum spin system like the J1-J2 Heisenberg Spin-1/2 model on the square lattice. Despite decades of research, certain aspects of its phase diagram remain unclear. Magnetic order can be established from the spin 2-point function, but the 4-point function would be required to pin down a putative valence-bond-solid order, currently out of reach for the pseudo-fermion fRG method. Other applications could be the three-dimensional Pyrochlore lattice or Rydberg atom quantum simulators which feature long-range interactions.

Further details

- Prerequisites: Condensed matter field theory, statistical physics, coding skills (C++ or python or julia).
- The project is expected to involve roughly 40% analytical and 60% numerical work.



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