Master project: **From Ising- to Heisenberg spins via functional renormalization**

Supervisor: Dr. Björn Sbierski [BJOERN.SBIERSKI@UNI-TUEBINGEN.DE]
Co-Supervisor: Prof. Dr. Igor Lesanovsky [IGOR.LESANOVSKY@UNI-TUEBINGEN.DE]

Institut für Theoretische Physik, Universität Tübingen, Nov. 2023

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 form like in the case of the paradigmatic quantum Heisenberg model,

$$H = \sum_{(i,j)} J_{(ij)} \mathbf{S}_i \cdot \mathbf{S}_j .$$

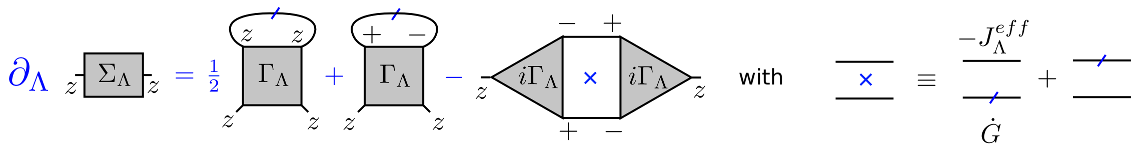
The majority of theoretical insights rest on numerical approaches based on matrix-product variational wavefunctions or quantum Monte Carlo (MC) simulations. However their performance is poor when it comes to three spatial dimensions or frustrated systems, respectively. In order to cope with these challenges, diagrammatic approaches to quantum spin systems have been pursued in the Matsubara formalism. One possibility is to represent spin-1/2 operators by a (pseudo-)fermion bilinear and treat the resulting interacting fermionic Hamiltonian by the functional renormalization group (fRG) method, see Ref. [3] for a recent review.

Despite certain merits of the described method, the representation of spin operators with auxiliary fermions has serious drawbacks like 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 [4] that directly works with spin correlation functions without taking a detour via auxiliary particle representations. This approach also allows for flexible schemes to define the RG flow. Ongoing work by the supervisor follows the idea to switch on the exchange coupling $J \rightarrow J_\Lambda \equiv \Lambda \cdot J$ with Λ being increased from zero (free spins) to unity. Alternatively, this scheme can be understood as decreasing the overall temperature from infinity. At the initial scale, correlation (and vertex-) functions are those of a free spin with highly non-trivial quantum dynamics.

The proposed project explores an alternative ansatz for the flow in spin-fRG: Deforming the Heisenberg- to the XXZ-model

$$J_{(ij)} \mathbf{S}_i \cdot \mathbf{S}_j \rightarrow J^z_{(ij)} S^z_i \cdot S^z_j + J^\perp_{(ij)} (S^x_i S^x_j + S^y_i S^y_j)$$

the idea is to use only $J^\perp \rightarrow J^\perp_\Lambda \equiv \Lambda \cdot J^\perp$ as the flow parameter. The starting point of the flow (at $\Lambda = 0$) is the classical Ising model for which correlation functions can be efficiently calculated using MC procedures [5]. This allows for a highly correlated yet classical starting point to which quantum fluctuations are added by the fRG. The main challenge will be to find reasonable truncation schemes such that the approximated flow is both precise and numerically tractable to as large Λ as possible.



Project roadmap

- Preparation: Familiarize yourself with the basic idea of the fRG [6], [7], then understand the spin-fRG formalism developed in [4] and the currently developed simplifications which will be provided as a set of notes from your supervisor. With help of local expertise build up a classical MC scheme that can provide low-order correlators for a simple benchmark model like the square-lattice Ising model.

- Flowing quantum fluctuations: Perform a symmetry analysis for correlation and vertex functions of XXZ spin models and derive the flow equations analytically. Set up a computer program that solves these flow equations. You will get support (and high-performance computing cluster access in Jülich) by your supervisor. To check the quality of the method, first apply it to the XXZ-dimer (just two spins) which can be solved analytically. Then proceed to extended but unfrustrated (e.g. ferromagnetic or bipartite) models where error-controlled quantum MC benchmark data is available in the literature.

- Application on 3d pyrochlore lattice: As a final application beyond the reach of quantum MC, use the developed formalism to study the effect of quantum fluctuations on the famous spin-ice model [8]. What type of phase transitions (if any) appear when you increase $J^\perp_{(ij)}$? Can you confirm the conjectured valence-bond phase [9] at the anti-ferromagnetic Heisenberg point?

Further details

- Prerequisites: Condensed matter field theory, statistical physics, coding skills (python/julia preferred).
- The project is expected to involve roughly 40% analytical and 60% numerical work.
- For reference: Recently completed MSc thesis with Björn Sbierski at LMU Munich by: Samira Hatoum (SAMIRA.HATOUM@LMU.DE) and Frederic Bippus (FREDERIC.BIPPUS@LMU.DE)

---

1. L. Savary, L. Balents, *Rep. Prog. Phys.* **80**, 16502 (2017).
2. A. Scheie, N. E. Sherman, M. Dupont, *et al.*, *Nature Physics* (2021).
3. T. Mueller, D. Kiese, N. Niggemann, *et al.*, *arxiv*, 2307.10359.
4. J. Krieg, P. Kopietz, *Phys. Rev. B* **99**, 060403 (Feb. 2019).
5. A. W. Sandvik, presented at the AIP Conference Proceedings, vol. 1297, pp. 135–338.
6. P. Kopietz, L. Bartosch, F. Schuetz, *Introduction to the Functional Renormalization Group* (Springer, 2010).
7. W. Metzner, M. Salmhofer, C. Honerkamp, V. Meden, K. Schonhammer, *Rev. Mod. Phys.* **84**, 299 (Mar. 2012).
8. M. J. P. Gingras, P. A. Mcclarty, *Rep. Prog. Phys.* **77**, 56501 (2014).
9. R. Schafer, B. Placke, O. Benton, R. Moessner, *Physical Review Letters* **131**, 096702 (2023).