Master project: **Pseudo-Majorana diagrammatic Monte Carlo for frustrated spin systems**

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Introduction Quantum spin systems harbor a wealth of interesting phenomena and are intensively studied both experimentally and theoretically. For example, a current research focus is on spin liquid phases that lack magnetic order but are characterized by fractionalized quasiparticles and entanglement [1]. 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,

$$H = \sum_{(i,j)} J_{(ij)} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{1}$$

The majority of theoretical insight rests 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 systems with frustrated couplings. 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 $S^{x,y,z}$ by three Majorana fermion operators $\eta^{x,y,z}$ (per spin) via

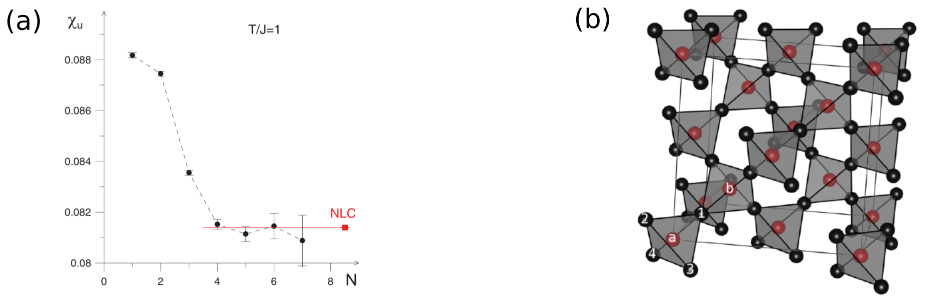
$$S^x = -i\eta^y\eta^z,\ S^y = -i\eta^z\eta^x,\ S^z = -i\eta^x\eta^y. \tag{2}$$

Majorana fermions can be thought as "half" an ordinary (complex-)fermion f and can be formally introduced as a hermitian combination of $f, f^\dagger$, i.e. $\eta \sim f^\dagger + f$ and $\eta' \sim i(f^\dagger - f)$.

Once the Heisenberg model is rewritten using the pseudo-Majorana (pm) representation (2) we obtain a purely interacting Majorana Hamiltonian. So far we have used the the functional renormalization group (fRG) to obtain correlation functions and thermodynamic quantities, see Ref. [2] for a recent review and in particular Refs. [3], [4]. Though generally successful, the pm-fRG method is currently limited to temperatures above $\sim 30\%$ of J. This is due to the necessary truncation of the per se exact hierarchy of fRG flow equations which, for the 4-point pm vertex, is only perturbatively correct to second order in J.

Despite the success of the diagrammatic resummation within the pm-fRG formalism (which allows to find critical temperatures with good precision) it would be desirable to explore diagrammatic expansions up to much higher order. This is possible via diagrammatic Monte Carlo (diagMC), which has recently enjoyed a major performance boost by the connected determinant (cDet) formalism [5]. The idea is to compute diagrammatic expansions stochastically using Monte Carlo methods, in this way expansions to order ~10 are achievable.

The proposed project explores the application of the cDet formalism for pm Hamiltonians. The goal is to implement and benchmark this novel simulation method and compare with existing approaches, in particular the pm-fRG. Is the pm-cDet approach superior when it comes to low temperatures? Does it outperform previous diagMC approaches to spin systems which neither employ the cDet idea nor the pm representation [6]?



Project roadmap

- Preparation: Familiarize yourself with the pm representation and the basic idea of Monte Carlo approaches. The classical Ising model is a good starting point to write your own code. Build on Ref. [7] and your group member's experience.

- pm-diagMC: Apply the cDet idea to interacting Majorana Hamiltonians. Start with the most simple case of four interacting Majoranas $H = V\eta_1\eta_2\eta_3\eta_4$ which can be solved analytically to test your approach and compute the first three orders in perturbation theory by hand, then apply CDet. Turning to pseudo-Majoranas, use the simple Heisenberg dimer $H = \mathbf{S}_1 \cdot \mathbf{S}_2$ as a benchmark model. Can your method beat the pm-fRG? You will receive existing notes in form of an internship report as guidance.

- Application to extended spin systems: As a final application apply the pm-diagMC to infinite spin systems in 1, 2 or 3 dimensions. First, models with exact numerical solutions like the XY chain can be considered for testing. Second, consider the triangular lattice which has been treated with pseudo-fermionic diag-MC before, see Fig. (a) for the convergence of the uniform susceptibility in diagram order from Ref. [6]. Is the pm-diagMC superior? If these tests are successful, apply your method to reveal new physics in complicated 3d models, for example find the temperature phase diagram of the *quantum* Heisenberg model on the centered Pyrochlore lattice [8], see Fig. (b). Spin models realized in state-of-the art Rydberg atom array experiments could be another target.

Further details

- Prerequisites: Condensed matter field theory, statistical physics, coding skills (python/julia preferred).
- The project is expected to involve roughly 50% analytical and 50% numerical work. High-performance computing resources will be provided if required.
- The research will be done in collaboration with Michel Ferrero (École Polytechnique, France) who is an expert in diagMC.
- 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)

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1. L. Savary, L. Balents, *Rep. Prog. Phys.* **80**, 16502 (2017).
2. T. Mueller, D. Kiese, N. Niggemann, *et al.*, *arxiv*, 2307.10359.
3. N. Niggemann, B. Sbierski, J. Reuther, *Phys. Rev. B* **103**, 104431, issn: 2469-9950, 2469-9969 (Mar. 2021).
4. N. Niggemann, J. Reuther, B. Sbierski, *SciPost Phys.* **12**, 156, issn: 2542-4653 (May 2022).
5. R. Rossi, *Physical Review Letters* **119**, 045701 (2017).
6. S. A. Kulagin, N. Prokof'ev, O. A. Starykh, B. Svistunov, C. N. Varney, *Phys. Rev. Lett.* **110**, 070601 (2013).
7. A. W. Sandvik, presented at the AIP Conference Proceedings, vol. 1297, pp. 135–338.
8. R. P. Nutakki, L. D. C. Jaubert, L. Pollet, *SciPost Physics* **15**, 040 (Aug. 1, 2023).