Numerical methods for simulating quantum skyrmions

Supervisor: Vahid Azimi Mousolou and Davoud Mirzaei

Division of Scientific Computing, Department of Information Technology, Uppsala University.

davoud.mirzaei@it.uu.se

Division of Materials Theory, Department of Physics and Astronomy, Uppsala University

vahid.azimi-mousolou@physics.uu.se

1 Introduction

Skyrmions (illustrate in Fig. 1) are topological solitons that emerge in various physical contexts. Their dynamics offer insights into the broader field of topological phases of matter, with potential applications in quantum materials, quantum spintronics, and quantum information processing. While skyrmions are widely discussed in classical magnetic textures, several studies have predicted the quantum behavior of skyrmions and their potential use as topologically protected quantum bits (qubits) [2, 3].

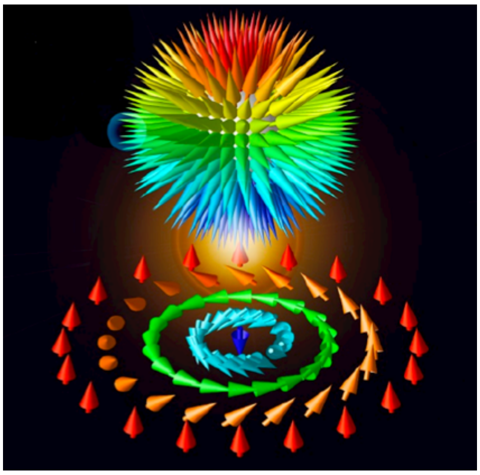

Figure 1: (Color online) Intuitive picture of the magnetic skyrmion [1].

2 Project Objectives

The quantum Landau–Lifshitz–Gilbert (LLG) equation, as proposed in [4], can be adapted to describe the dynamics of quantum skyrmions, accounting for both their coherent precession and dissipative effects within a quantum framework. While the LLG equation is well-established for classical skyrmions, extending it to the quantum regime requires additional considerations to capture essential quantum phenomena such as coherence, fluctuations, and quantum correlations. Understanding these dynamics is crucial in the fields of condensed matter physics and quantum information science. This project aims to develop and implement numerical methods for simulating quantum skyrmions by solving the quantum LLG equation [4]. In the computational side we aim to develope efficent numerical algorithms for solving

$$\rho' = \frac{i}{\hbar}[\rho, H] + i\kappa[\rho, \rho'], \quad \rho(t=0) = \rho_0,$$

where ρ is the density matrix of size N with complex entries, H is the Hamiltonian, $\hbar$ is the Planck constant, κ is a dimensionless damping rate, and ρ_0 is the initial state. Here $[\cdot, \cdot]$ is the commutator of two operators defined as $[A, B] = AB - BA$.

The challenges in solving this equation arise from several factors. First, the density ρ is represented as a matrix, unlike in classical equations where the density is a vector. Second, the presence of the additional damping term $i\kappa[\rho, \rho']$ introduces a significant nonlinearity into the system. Finally, the large value of N, which is typically on the order of 2^n where n is the number of spins (qubits), further complicates the problem due to the exponential growth in the system's size.

The student will focus on algorithm development and numerical simulations to investigate how quantum effects influence the stability and dynamics of skyrmions in nanoscale systems.

3 Planed tasks and required expertise

Planed tasks are:

- Learning and understanding the model systems and equations describing quantum skyrmoins,
- Developing an efficient numerical ODE solver for the quantum LLG model,
- Enhancing the algorithm for large scale problems

The required backgrounds are:

1. Basic understanding of numerical methods for ODEs,
2. Basic understanding of matrix computations,
3. Computer programming with basic understanding of HPC
4. Willingness to learn about numerical methods and quantum information processing.

References

[1] Y. Tokura, and N. Kanazawa, Magnetic skyrmion materials, Chemical Reviews 121(5), 2857-2897 (2020).

[2] H. Ochoa and Y. Tserkovnyak, Quantum skyrmionics, Int. J. Mod. Phys. B 33, 1930005 (2019).

[3] C. Psaroudaki and C. Panagopoulos, Skyrmion qubits: a new class of quantum logic elements based on nanoscale magnetization, Phys. Rev. Lett. 127, 067201 (2021).

[4] Y. Liu, I. P. Miranda, L. Johnson, A. Bergman, A. Delin, D. Thonig, M. Pereiro, O. Eriksson, V. Azimi-Mousolou, and E. Sjöqvist, Quantum analog of Landau-Lifshitz-Gilbert dynamics, arXiv:2403.09255.