1. Semester Report

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Ph.D. Thesis title: Molecular magnets for quantum technology applications

January 31, 2025

Introduction

Recent advances in quantum materials research have highlighted the potential of skyrmions - topologically protected magnetic structures - for next-generation computing architectures. These magnetic quasi-particles are particularly promising for developing low-energy, non-volatile memory devices due to their stability and controllability. Our research leverages density functional theory (DFT) calculations using the SIESTA code, which implements a Linear Combination of Atomic Orbitals (LCAO) approach. While performing DFT calculations has become relatively straightforward, the critical challenge lies in extracting meaningful magnetic parameters from these calculations. Recent methodological advances have now made it possible to systematically derive parameters for the general Heisenberg model from DFT results, opening new avenues for magnetic systems research. This breakthrough in parameter extraction enables us to bridge the gap between quantum mechanical calculations and magnetic structure prediction. By accurately determining the magnetic interaction parameters, we can first perform reliable spin dynamics simulations using the Landau-Lifshitz-Gilbert equation and then predict conditions under which skyrmions might form in different materials. Finally we can evaluate the stability and behavior of these magnetic structures.

Research work carried out in current semester

We used the theoretical framework developed in the paper 'Relativistic magnetic interactions from non-orthogonal basis sets'[1]. It describes a method that allows us to extract the interaction parameters for the generalized Heisenberg Hamiltonian describing spin-spin interactions

$$H(\{\mathbf{S}_i\}) = \frac{1}{2}\sum_{i\neq j}\mathbf{S}_i\mathcal{J}_{ij}\mathbf{S}_j + \sum_i \mathbf{S}_i\mathcal{K}_i\mathbf{S}_i \tag{1}$$

where $\mathcal{J}_{ij}$ represents the exchange coupling between spins and $\mathcal{K}_i$ denotes the intra-atomic magnetic anisotropy. Then we can compare energy variations upon rotations expanded to second order in the Heisenberg Hamiltonian

$$E_A^1(\{\mathbf{o}\},\mathbf{u}_A) = \frac{1}{2}\left(\mathbf{o}\left(\sum_i J_{iA} + 2K_A\right)\mathbf{o}_A^1 + \mathbf{o}_A^1\left(\sum_i J_{Ai} + 2K_A\right)\mathbf{o}\right), \tag{2}$$

$$E_A^2(\{\mathbf{o}\},\mathbf{u}_A) = \frac{1}{2}\left(\mathbf{o}\left(\sum_i J_{iA} + 2K_A\right)\mathbf{o}_A^2 + \mathbf{o}_A^2\left(\sum_i J_{Ai} + 2K_A\right)\mathbf{o}\right) + \mathbf{o}_A^1 K_A \mathbf{o}_A^1, \tag{3}$$

where $\mathbf{o}$ is the direction of the parallel or antiparallel spins and $\mathbf{u}$ defines the rotation axis, to the energy variations upon rotations from the Kohn-Sham Hamiltonian given by the DFT calculation. These energies can be computed using the LKAG torque method.

$$\delta E_A^{KS} = \int_{-\infty}^{E_F} d\epsilon\, \epsilon \delta\rho_A(\epsilon) = -\frac{1}{\pi}\int_{-\infty}^{E_F} d\epsilon\, \mathrm{Im\,Tr}\ln(\hat{I} - \hat{V}_A\hat{G}_0(\epsilon)), \tag{4}$$

where $\hat{V}_A$ is the local perturbation caused by the rotation and $\hat{G}_0(\epsilon)$ is the Green's function of the Hamiltonian.

We implemented these methods in a Python library that handles magnetic entity creation across multiple scales, from individual atoms or atomic shells to clusters of atoms. The library generates magnetic pairs based on a cutoff radii for the interaction and on a possible list of conditions that can be passed. Our primary contribution lies in the optimization and parallelization of these calculations. We use MPI for distributed computing across clusters and developed GPU acceleration techniques for computationally intensive operations. This enhanced computational capability enabled us to analyze systems with very large unit cells. We are validating our results through multiple systems, including Fe3GeTe2, variously built isolated equilateral chromium trimers and a large systems with a layer of two-dimensional tungsten diselenide and chromium triiodide, using SIESTA calculations.

The investigation on the smaller systems revealed crucial insights about system symmetry and the importance of atomic positions on finite grids. These factors can create significant variations in calculated parameters, highlighting the necessity for precise positioning and careful symmetry considerations.

Through our high-performance computing approach, we presented that we can extract parameters from a unit cell of 243 atoms. This work represents an advancement in magnetic parameter calculation for larger systems and layered 2D materials.

Publication

During this semester, the primary focus was on developing new computational capabilities. The paper extending my master's thesis, "Magnetic properties of graphene triangulenes embedded in hexagonal boron-nitride," is expected to be ready for submission by the end of next semester. The new computational methodologies developed during this period have opened up possibilities for studying previously inaccessible systems, potentially leading to additional publications in the coming year. The work on quantum reservoir computing was progressing slower than expected; at this time, it is unclear when it can be published, but it should be in focus for the next semester.

Studies in current semester

During the semester, I completed two courses that directly support my research objectives:

- **Quantum bits in solids (FIZ/1/041E)**
- **Classical and Quantum Optimization (FIZ/3/097)**

Conferences in current semester

I participated in several significant academic events this semester:

- Graphene workshop at Budapest University of Technology and Economics, Hungary
- TRILMAX kickoff meeting at Eötvös Loránd University, Hungary
- QUEST kickoff meeting at Eötvös Loránd University, Hungary
- Advancing Quantum Theory for Future Quantum Technologies at Linköping University, Sweden

Teaching activity in current semester

I served as an instructor for the Data Mining and Machine Learning course (dsminingf17vm), which introduces fundamental machine learning concepts to bachelor and master students. My responsibilities were the supervision of multiple projects and the grading of the final reports.

Acknowledgments

This research has been made possible through the support of two Horizon Europe projects, QUEST and TRILMAX. These initiatives have provided invaluable opportunities for conference attendance and professional development within a collaborative research environment. I gratefully acknowledge the computational resources provided by KIFÜ in Hungary and NAISS in Sweden, which have been essential for conducting our numerical simulations and analyses.

References

[1] Gabriel Martínez-Carracedo et al. "Relativistic magnetic interactions from nonorthogonal basis sets". In: *Physical Review B* 108.21 (2023), p. 214418.