2. Semester Report

Dániel Tibor Pozsár (danielpozsar@ttk.elte.hu)
PhD program: Statistical Physics, Biological Physics and Physics of Quantum Systems
Supervisors: Viktor Ivády, László Oroszlány
Ph.D. Thesis title: Molecular magnets for quantum technology applications

June 23, 2026

Introduction

As described in the first-semester report, the methodological backbone of this work is the first-principles extraction of the parameters of the generalized relativistic Heisenberg Hamiltonian from density functional theory (DFT), followed by their use in finite-temperature spin simulations. To this end, in the first semester I began developing `grogupy`, a Python implementation of the Liechtenstein–Katsnelson–Antropov–Gubanov (LKAG) torque method generalized to the non-orthogonal basis sets, like in SIESTA based on an earlier paper [1]. The present semester was devoted to three goals: (i) maturing `grogupy` into a robust, parallel and well-tested research package; (ii) completing and presenting a spin model of graphene triangulenes embedded in hexagonal boron nitride (hBN); and (iii) continuing the quantum reservoir computing (QRC) work based on nitrogen-vacancy (NV^-) centers in diamond.

Research work carried out in current semester

The modeling target is the generalized relativistic Heisenberg Hamiltonian, written in the decomposed form

$$H(\{\mathbf{e}_i\}) = \frac{1}{2}\sum_{i\neq j} J_{ij}^{\mathrm{iso}}\,\mathbf{e}_i\cdot\mathbf{e}_j + \frac{1}{2}\sum_{i\neq j}\mathbf{e}_i\,\mathcal{J}_{ij}^{S}\,\mathbf{e}_j + \frac{1}{2}\sum_{i\neq j}\mathbf{D}_{ij}\cdot(\mathbf{e}_i\times\mathbf{e}_j) + \frac{1}{2}\sum_i \mathbf{e}_i\,\mathcal{K}_i\,\mathbf{e}_i, \quad (1)$$

where J_{ij}^{iso} is the isotropic exchange, $\mathcal{J}_{ij}^{S}$ the symmetric anisotropic exchange, $\mathbf{D}_{ij}$ the Dzyaloshinskii–Moriya (DM) vectors and $\mathcal{K}_i$ the single-ion anisotropy. These are obtained by matching the energy variations of Eq. (1) under controlled spin rotations to those of the Kohn–Sham Hamiltonian, evaluated with the LKAG torque expression

$$\delta E_A^{\mathrm{KS}} = -\frac{1}{\pi}\int_{-\infty}^{E_F} d\epsilon\ \mathrm{Im}\,\mathrm{Tr}\,\ln\big(\hat{I} - \hat{V}_A\hat{G}_0(\epsilon)\big), \quad (2)$$

with $\hat{V}_A$ the local rotation-induced perturbation and $\hat{G}_0(\epsilon)$ the Green's function of the unperturbed Hamiltonian.

`grogupy` **development.** The library was consolidated into a documented, installable Python package with a unified magnetic-entity construction API spanning individual atoms, atomic shells and clusters of atoms; magnetic pairs are generated automatically from interaction cutoff radii together with user-supplied conditions. I implemented and validated the anisotropy-tensor fitting routines that extract J^{iso}, $\mathcal{J}^S$, $\mathbf{D}_{ij}$ and $\mathcal{K}_i$ from the rotated-spin energy landscape, and consolidated the MPI-distributed and GPU-accelerated backends for the Green's-function–intensive steps, enabling unit cells of a few hundred atoms. Outputs were cross-validated against independent reference implementations, and I continued the dialogue with the original authors of the method regarding integration-contour boundaries and SIESTA numerical-precision differences.

Triangulenes in hBN. I completed the spin model of graphene triangulenes embedded in hBN (an extension of my MSc thesis) and presented it to international audiences (see below).

Quantum reservoir computing with NV^- centers. I continued the QRC simulations using the negatively charged nitrogen-vacancy (NV^-) center in diamond as the physical reservoir, working toward a quantum state-recognition task.

Studies in current semester

No ELTE lecture courses were registered this term. As accepted summer-school participation I attended the

- **Aalto/Helsinki Summer School on New Directions in Quantum and Quantum Reservoir Computing** (Aalto University, Finland, 18–23 Aug 2025).

Conferences in current semester

- DPG Spring Meeting (Condensed Matter Section), Regensburg, Germany, 15–22 Mar 2025 — **contributed talk MA 8.6** on the triangulene/hBN spin model.
- COST Action CA23134 "Polytopo" (Physics and Mathematics of Topological Textures), BME, Budapest, 14–16 May 2025.
- *Let's give it a spin!*, Belgrade, Serbia, 20–23 May 2025 — **oral talk** on the triangulene/hBN spin model.
- CECAM conference, Toulouse, France, 24–28 Jun 2025 — **poster** on the triangulene work.
- Research visit to Valencia ($NiBr_2$ work), Spain, 14–27 Jul 2025.

Departmental and consortium seminars: internal TRILMAX and QRC presentations during the term.

Teaching activity in current semester

Numerical Methods in Physics — exercise instructor. This teaching contribution was not separately credited.

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.