3. Semester Report

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Introduction

Building on the previous semesters, in which `grogupy` reached maturity, this semester delivered its first full application — the relativistic-exchange study of the CrI_3/WTe_2 heterostructure — with further applications now in preparation. In parallel I started two new projects: a simulation of the coherence time of the V_B^- center in hBN, carried out with other ELTE PhD students, and, together with the Loughborough group, a quantum-reservoir-computing study based on transverse-field Ising model (TFIM) reservoirs, alongside the ongoing nitrogen-vacancy (NV^-) QRC work within the consortium.

Research work carried out in current semester

CrI_3/WTe_2: the first application of `grogupy`. This semester `grogupy` reached its first full application, with further applications already in preparation. Using the fully relativistic DFT + `grogupy` pipeline, we computed the relativistic exchange parameters of monolayer CrI_3, both isolated and proximity-coupled to metallic WTe_2. Isolated CrI_3 is a magnetic semiconductor governed by superexchange, with an experimental Curie temperature $T_C \approx 45$ K. On WTe_2 the CrI_3 layer becomes metallic, yet there is no major electronic reconstruction, the effect is a pure relativistic proximity effect. The range of the isotropic exchange J^{iso} increases and the magnetic anisotropy changes direction; quantitatively, the magnetocrystalline anisotropy energy switches sign,

$$\Delta E = E_{\text{IP}} - E_{\text{OOP}} = \begin{cases} +0.94 \text{ meV/cell}, & \text{isolated } CrI_3 \text{ (OOP easy axis)}, \\ -0.35 \text{ meV/cell}, & CrI_3/WTe_2 \text{ (IP easy axis)}, \end{cases} \tag{1}$$

i.e. a proximity-induced spin reorientation from out-of-plane (OOP) to in-plane (IP). Feeding the extracted parameters into VAMPIRE Monte Carlo simulations [1] of the relativistic Heisenberg model yields

$$T_C = 23.5 \text{ K } (CrI_3, \text{ OOP}) \rightarrow 33.0 \text{ K } (CrI_3/WTe_2, \text{ OOP}),\ 34.0 \text{ K } (CrI_3/WTe_2, \text{ IP}),$$

a 40–50% enhancement of T_C. The work was coordinated through recurring Budapest–Oviedo TRILMAX meetings with Z. Tajkov, J. Ferrer and A. García-Fuente, and a dedicated discussion with E. Navarro-Moratalla, Z. Tajkov and L. Oroszlány.

Coherence of the V_B^- center in hBN. Together with other PhD students from ELTE, we initiated an *ab initio*-informed simulation of the coherence time T_2 of the V_B^- ($S = 1$) center in hBN, including the spin-bath composition, dynamic decoupling, and sample-thickness dependence. The model starts from the total Hamiltonian

$$H = H_{V_B} + H_{\text{int}} + H_{\text{bath}}, \qquad H_{\text{bath}} \approx H_{\text{spin-1/2}} + H_{\text{spin-1}} + H_{\text{nuc}}, \tag{2}$$

with the central spin coupled to a mixed bath of electronic spin-1/2, electronic spin-1, and nuclear-spin species. We set up the cluster-correlation expansion (CCE) framework, using `pyCCE`, for the Hahn-echo coherence function $\mathcal{L}(t)$ and started exploratory simulations.

Quantum reservoir computing. Within the weekly QRC consortium theory meetings (with the Loughborough/LiU/Aalto/Montpellier/Leibniz-IPHT partners, organized by A. Zagoskin) we progressed a great deal on the NV^--based quantum reservoir computing. In addition, together with the Loughborough researchers I started a new QRC project based on transverse-field Ising model (TFIM) reservoirs.

Studies in current semester

- Topological Insulators I (FIZ/1/042E) — Satisfactory.
- Extremes, Records, and Order-Statistics in Nature (FIZ/3/075E) — Excellent.

Conferences in current semester

- TRILMAX Theory Summer School, Oviedo, Spain, 7–12 Sep 2025 — attended as **invited tutor**, delivering lectures on `grogupy`.
- Loughborough research stay — 28 Sep – 1 Nov 2025.

Teaching activity in current semester

Computer Science Fundamentals, first-year BSc — exercise instructor (FIZ/OKT/2, completed).

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References

[1] Fried-Conrad Weber et al. “Atomistic spin dynamics with quantum colored noise”. In: *arXiv preprint arXiv:2508.11315* (2025).