Skoltech
Skolkovo Institute of Science and Technology

Jury Member Report – Doctor of Philosophy thesis.

Name of Candidate: Grigory Starkov

PhD Program: Physics

Title of Thesis: Simulations of high temperature spin dynamics

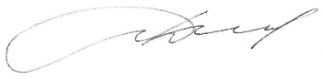
Supervisor: Assistant professor Anatoly Dymarsky

Co-advisor: Associate professor Boris Fine

Chair of PhD defense Jury: Professor Anton Andreev ***Email****: An.Andreev@skoltech.ru*

Date of Thesis Defense: 16 October 2019

Name of the Reviewer: Professor Vladimir Drachev

I confirm the absence of any conflict of interest	**Signature:**  **Date: 18-09-2019**

The purpose of this report is to obtain an independent review from the members of PhD defense Jury before the thesis defense. The members of PhD defense Jury are asked to submit signed copy of the report at least 30 days prior the thesis defense. The Reviewers are asked to bring a copy of the completed report to the thesis defense and to discuss the contents of each report with each other before the thesis defense.

If the reviewers have any queries about the thesis which they wish to raise in advance, please contact the Chair of the Jury.

Reviewer's Report

Reviewers report should contain the following items:

- Brief evaluation of the thesis quality and overall structure of the dissertation.
- The relevance of the topic of dissertation work to its actual content
- The relevance of the methods used in the dissertation
- The scientific significance of the results obtained and their compliance with the international level and current state of the art
- The relevance of the obtained results to applications (if applicable)

- The quality of publications

The summary of issues to be addressed before/during the thesis defense

The thesis is focused on the theoretical approach to dynamics of nuclear spins in solids in context of the techniques of Nuclear Magnetic Resonance (NMR). The authors develop a hybrid quantum-classical method for first-principles calculations of spin dynamics. The method is based on dividing the lattice of quantum spins into a central quantum cluster and an environment. The environment is approximated then by classical spins. The quantum cluster and the classical environment interact by exerting effective magnetic fields on each other.

The method is applied to the calculations of Free Induction Decay (FID) in the context of NMR. FID is the observable NMR signal generated by non-equilibrium nuclear spin magnetization precessing about the magnetic field. This non-equilibrium magnetization can be induced, generally by applying a pulse of resonant radio-frequency close to the Larmor precession frequency of the nuclear spins. The FID signal is typically measured in experiments. Hybrid method's predictions are compared with directly computed FIDs for various one- and two-dimensional models, and with experimentally measured FIDs for real materials, such as CaF2, 29Si-enriched silicon and calcium fluorapatite Ca10(PO4)6F2. In almost all cases considered, excellent performance of the hybrid method is observed.

The dissertation is reasonably structured. It starts with the introduction, where all the related experiments and the literature models are discussed. It continues with Chapter 2, which introduces key theoretical ideas. Note at this point, that Chapter 2 should be added by a paragraph clearly explaining whether it contains anything new relative to the literature.

Chapters 3-5 describe the core of the dissertation. Namely, the author presents here the hybrid method, which then applied to the calculation of correlation function and FID to compare with experiments and other models. The dissertation contains some supplementary sections providing important details.

I have not found real issues. The method implies approximation, which reflects better experiments on FID compared with other methods in some difficult cases like 29Si-enriched silicon and calcium fluorapatite Ca10(PO4)6F2. However, as far as I understand, the hybrid method works worse than the classical approach for CaF2, see Table 5.1. It would be desirable to discuss the reason for difference in the method applications between different materials.

As I mentioned above it would be great if Chapter 2 will be added by a paragraph clearly explaining whether the narratives contain anything new relative to the literature.

The results were published in two high quality papers in worldwide recognized journals, Physical Review B and The European Physical Journal Special Topics. This fact itself indicates scientific significance of the results and their compliance with the international level.

To summarize, this dissertation can be considered as a well done work and the author deserves PhD degree without any reservations.

Provisional Recommendation
I recommend that the candidate should defend the thesis by means of a formal thesis defense