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: E.B. Fel'dman

I confirm the absence of any conflict of interest	**Signature:**  **Date: 15-09-2019**

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

Doctoral thesis of G.Starkov is focused on the dynamics of spins coupled by the dipole-dipole interactions (DDI) in solids at high temperatures. That dynamics is closely connected with Free Induction Decay (FID) which is one of the main observables in Nuclear Magnetic Resonance (NMR). The line shape of NMR and its Fourier transform, the FID, are very important sources of information about the structure and dynamics in condensed matter. At the same time, the problem of the line shape in solids is intimately connected with the fundamental problem of statistical physics – the establishment of equilibrium in a many-particle system. Without any doubts, the topic of the doctoral thesis is relevant and important.

That problem has been studied by many physicists for a long time, however, an exhaustive solution was not obtained. Among previous achievements I note the Abragam's formula which is based on an introduction of nearest and remote spins. Spin dynamics of the nearest spins is investigated exactly. The remote spins create on a given spin a random local field. The distribution of the random local fields is a Gaussian one, according to the central limit theorem of the probability theory. That approach does not take into account the correlations of the remote spins. As a result, it leads to some discrepancies between experimental data and theoretical predictions. B. N. Provotorov, A. A. Lundin, V.E. Zobov developed the approach which was suggested by A.Abragam. However they did not take into account the interactions between nearest and remote spins.

In this thesis the author develops a hybrid quantum-classical method for first-principles calculations of high- temperature spin dynamics. The author suggested to divide the lattice of quantum spins into a central quantum cluster and an environment which is approximated by classical spins. It is very important that in the suggested model the quantum cluster and the classical environment interact by exerting effective magnetic fields on each other. The author performs a detailed comparison of the results obtained by the described method with experimentally measured FIDs for real materials, such as CaF_2, ^{29}Si-enriched silicon and calcium fluorapatite $Ca_{10}(PO_4)_6F_2$, and obtained a very good agreement.

The title of thesis reflects its content The text of the thesis is written clearly.The scientific level of the thesis corresponds to the state of the art in the considered field.

I believe that the methods developed in the thesis are original and very useful for statistical physics and NMR spectroscopy.

Provisional Recommendation

☒ *I recommend that the candidate should defend the thesis by means of a formal thesis defense*

☐ *I recommend that the candidate should defend the thesis by means of a formal thesis defense only after appropriate changes would be introduced in candidate's thesis according to the recommendations of the present report*
☐ *The thesis is not acceptable and I recommend that the candidate be exempt from the formal thesis defense*