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:

I confirm the absence of any conflict of interest (Alternatively, Reviewer can formulate a possible conflict)	**Signature:** 15/09/2019 **Date: DD-MM-YYYY**

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 devoted to the study of nuclear spin relaxation in nonmagnetic crystalline dielectrics. This is a very important subject, which has been studied extensively. The main result of the thesis is a hybrid method of quantum simulation of the problem of relaxation of total nuclear magnetization of the sample. In this approach, only a small number of spins in the system are treated quantum mechanically, while the others are treated classically. This enables simulating much larger samples than would be possible in a full quantum simulation. Extensive simulations based on this method were performed. Their results were compared with experimental data on several compounds, and were generally in good agreement. This work has resulted in two publications in reputable journals.

The thesis is clearly written. It provides a good introduction into the huge field of nuclear spin relaxation and summarizes relevant prior work. All the important assumptions and approximations are explicitly stated.

My main question concerns the justification of the method. The influence of the quantum cluster on the classical spins is described by a rescaled average (over the state of the quantum cluster) of the interaction Hamiltonian. Ideally, I would like to see a better microscopic justification of this procedure. Nevertheless, even in the absence thereof I recommend the thesis to proceed to formal defense. Many very useful numerical method lack microscopic justification.

There are several typos that I would like mention.

Page 1, fourth line from the bottom in first paragraph; fix ``than then the ones"

Page 2, last line; replace ``momentum" with ``moment"

Above (1.24); fix ``this rapidly oscillating terms"

Page 16, mid-page; ``higher then"

Eq. (1.74): fix subscript of the quantum state in the left hand side.

Line above (1.76); remove ``relative"?

I also have a few Optional suggestions:

Line below Eq. (1.6); I would remove the word ``initial"

Paragraph below (1.9); I found the description of the relaxation times T_1 and T_2 here a bit confusing. Perhaps it would be better to state the conventional definition in terms of relaxation rates of the longitudinal and transverse magnetization.

The paragraph immediately below it; I suggest explicitly stating that NONMAGNETIC dielectrics are considered.

Paragraph above (1.11); I suggest replacing ``fluctuating'' with ``time dependent''.

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*