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:** A. Polkovnikov 09-08-2019 **Date: DD-MM-YYYY**

Reviewer's Report

This thesis focuses on developing a quantum-classical hybrid method for simulating quantum dynamics of interacting spins in a typical NMR setup. The main idea behind the method is to treat a small but finite subset of spins exactly within the QM framework and treat a much larger collection of spins, which are outside this subset as (semi)-classical objects. This thesis nicely demonstrates that in various situations of experimental relevance this newly developed method results in significant improvements over both the size limited exact diagonalization and the traditional semiclassical approach. One chapter of the thesis focuses on the analysis of the method in some model situations and another chapter analyzes a specific, experimentally relevant, setup making direct comparisons of theory with the experimental data. I personally find both the structure of the dissertation and the quality of presentation to be excellent.

The topic of the dissertation exactly matches its content.

The dissertation is essentially split in two parts: i) developing a new method and ii) applications of the method. In this sense the methods are of course relevant to the dissertation. In principle, one could argue that there are other recently developed numerical methods available now. So one could add some at least qualitative discussions of the relevance of those, but I think the dissertation is self-contained as is.

The addressed problem is very difficult and is in the heart of very active research both experimental and theoretical. So the methods might find many various applications in future. Results demonstrated in the thesis are beyond reach of standard methods, so I have little doubts that they are very valuable. As I wrote more comparisons with other techniques could be useful, but this could (and likely will) be done in future and likely optimized methods will emerge. I see a lot of future of the particular idea developed in this thesis.

Chapter 5 of this thesis is exclusively devoted to applications of these methods to real materials demonstrating that the results are highly relevant to explaining existing experiments.

The work of the thesis is based on two publications in refereed international journals (Phys. Rev. B and The European Physical Journal Special Topics).

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*