Skoltech
Skolkovo Institute of Science and Technology

Thesis Changes Log

Name of Candidate: Grigorii Starkov

PhD Program: Physics

Title of Thesis: Simulations of High-Temperature Spin Dynamics

Supervisor: Prof. Boris Fine, Prof. Anatoly Dymarsky

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

Date of Thesis Defense: 16 October 2019

The thesis document includes the following changes in answer to the external review process.

Dear Jury Members,

I am truly grateful to you for your effort in careful reading of the thesis.

Thank you for your useful comments and for the suggestions in improving the quality of the dissertation.

In response to your reviews, I have made the following modifications in the final version of the text.

Reviewer: Prof. Anton Andreev

- *"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."*

Answer: The rescaling procedure guarantees that the initial behaviour of a hybrid lattice is identical to that of the quantum lattice. Additionally it guarantees that the hybrid method works well in the limit of large effective number of interacting neighbours. Overall, however, we are unable to provide a rigorous mathematical justification.

In thesis, we have edited Section "Uncertainty estimate" at the end of Chapter 3 "The Hybrid Method".

- *"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"?"

  Answer: Thank you for your suggestions. We have fixed the listed typos.

- *"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."*

Answer: In paragraph below (1.9), we have added a footnote where we mention the conventional definitions of these time scales.

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

  Answer: we have done as you suggested.

- *"Paragraph above (1.11); I suggest replacing ``fluctuating" with ``time dependent"."*

  Answer: we replaced "fluctuating fields" with "fields fluctuating in space and time".

Reviewer: Prof. Alexei Buchachenko

- "*The author introduces (p.2) the units with the Boltzmann constant kB = 1. It looks a bit misleading, the more so β = 1/ kBT is always used in what follows."*

Answer: We have omitted introduction of units k_B=1 at the start of Section 1.2. The only place where we used the temperature T was Eq. (1.9). There, we re-expressed T in terms of β.

- *"Equation (1.9) is one of the cornerstone of the approach, which allows one to assume energy conservation on the timescale of spin relaxation. On the other hand, some arguments relying on the long-time limit (e.g., p.50) are used. Is it possible that long-time behavior of the measured FID curves would be affected by energy relaxation?"*

Answer: We define this long-time behaviour for the times t where T2<<t<<T1. In principle, energy relaxation slightly renormalizes the constant of long-time decay. However, since T2<<T1, this effect is negligible.

We have added a suitable commentary at the end of the second paragraph in Section 4.2 "Discussion".

- "*Chapter 2 essentially lacks the references. Is it well-known (for the happy few) or constitutes original results of the Thesis?"* (This question is identical to the one asked by Prof. Drachev)

Answer: To improve the clarity of presentation, we moved the derivations of first and second order tensors at the end of Section 2.1 into a separate Section (2.2). In the following, we list the changes in terms of new Section numbers.

We have added the references at the end of Section 2.1, at the beginning of Section 2.3 and at the end of the second paragraph in Section 2.6.

- "*In chapter 5, the choice of basic parameters is not specified for "real-materials applications". Apparently, gyromagnetic ratios were set for bare nuclei and spin-spin coupling constants are derived from them within the truncated magnetic dipolar approximation. Is this choice appropriate as the effective magnetic parameters in the real materials may be different? Are the results sensitive to the parameter choice?"*

Answer: bare nuclear gyromagnetic ratios are used throughout the thesis.

In order to emphasize this fact, we have added a footnote in the discussion after Eq. (1.10) and a comment at the end of the first paragraph in Section 5.1

- **"***Statistical uncertainty estimate appears on p.52 a bit unexpectedly. Perhaps it deserves some introduction and reference to Appendix A.3. By the way, it looks strange that the statistics of the Si and calcium fluorapatite simulation is not attested***."**

We have edited the second paragraph of Section 5.1 to better explain the appearance of the statistical uncertainty estimate. Also, we added there a reference to Appendix "Statistics behind the plots". In that Appendix, the table A.1 was split into two tables corresponding to the simulations of Chapters 4 and 5 respectively. The numbers of computational runs for Si and fluorapatite simulations were added to the second table.

- "*On p.59, fig. 5.8 comes out of order. Better place it together with the fig. 5.4".*

Answer: we placed old Fig. 5.8 between old Figs. 5.4 and 5.5. (Now, these are Figs. 5.5, 5.4 and 5.6 respectively).

- "*Throughout the Thesis, prohibitive complexity of the rigorous quantum simulations is repeatedly mentioned. It would be instructive to give examples of current limitations from literature or author's own experience."*

Answer: We have added penultimate paragraph to Section 1.4.2 where such examples are provided.

- *"I strongly recommend to rewrite Outlook section stressing on the perspectives which can be concisely and clearly justified on a base of the material presented in the Thesis. Other prospects can be considered as challenges, but the essence and reason of a challenge should be given."*

Answer: As it was suggested, we have completely rewritten Outlook section in order to address the mentioned problems.

- *"Despite the work is well and accurately written, quite a few misprints and formatting inaccuracies exist. E.g. Acknowledgments line 2, p.1 l.10, sec.1.2.3 l.6, p.23 l.2 (missing reference), p.34 l.4, p.38 l.7, p.43 l.25, etc.; behavior/behaviour, equation references with and without parentheses,... Careful proofreading should be helpful to eliminate these and other imperfections."*

Answer: We have fixed the listed misprints and formatting inaccuracies in addition to the ones we were able to identify ourselves.

Reviewer: Dr. Viatscheslav Dobrovitski

- "*First, it would be useful to comment on the number of the samples of the random function |psi> needed for accurate evaluation of the quantum correlation function (in purely quantum simulations, for sufficiently large systems, even a single sample would suffice while the current method requires many more samples)*".

Answer: We have edited the discussion after Eq. 1.76 to emphasize the fact that a single sample would suffice even for moderately large systems.

- "Second, it might be good to emphasize the difference between the method of Ref. 32, based on the calculation of <psi|A(t)|psi><psi|A|psi>, and the previously used method based on calculation of <psi|A(t)A(0)|psi>, and clarify the difference between the two."

Answer: We have added the relevant discussion at the end of Section 3.2.

Additionally, we have added Appendix A.2 "Scaling of statistical errors".

Reviewer: Prof. Anatoli Polkovnikov

- *"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 is self-contained as is."*

In penultimate paragraph of Section 1.5, we have added references to the papers on Cluster Truncated Wigner Approximation supplemented by a brief discussion.

Reviewer: Prof. Vladimir Drachev

- *"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."* (This question is identical to the one asked by Prof. Buchachenko.)

Answer: To improve the clarity of presentation, we moved the derivations of first and second order tensors at the end of Section 2.1 into a separate Section (2.2). In the following, we list the changes in terms of new Section numbers.

We have added the references to previous works at the end of Section 2.1, at the beginning of Section 2.3 and at the end of the second paragraph in Section 2.6. (These changes are the duplicates of the ones we listed in the answer to an identical question of Prof. Alexei Buchachenko.)

Reviewer: Dr. Eduard Feldman

No questions or suggestions to address.