TO: Dr. Helen Gray, Editor

Physical Chemistry Chemical Physics

Dear Dr. Helen Gray,

Thank you for your e-mail attached with the Referees' reports on our manuscript CP-PER-11-2011-023700. We thank the referees for the pertinent comments and useful suggestions, which help us improve our work significantly. We have answered the Referees' current queries and as well made some changes to the paper accordingly as follows.

Referee 1 wrote:

1. In most of the sections, the relevant issues have carefully been chosen and elaborately described for non-specialists, except for 2.2.2. Indeed, the references have been cited, but a more detailed description will be necessary for non-specialists.

Ans: We have rewritten 2.2.2 and added the form of the first-order Trotter-Suzuki formula to make it comprehensible for non-specialists.

2. In Fig. 4(b), the units description is not correct according to the IUPAC/IUPAP conventions.

Ans: We have changed the unit "Angstrom" in the x-axis to "\AA". Now the units description in Fig. 4(b) are the same as Fig. 1 in N. Doslic et al., J. Phys. Chem. A, 1998, 102 (47), 9645-9650.

Referee 2 wrote:

1. Thus, I decided to write the changes directly into the manuscript, so it would be easier to identify what to change and where to introduce the change.

Ans: We are very grateful to the Referee's specific suggestions, as these modifications over 200 times improve our manuscript significantly. We have nearly accepted all the suggestions and made some other necessary changes. We again thank the Referee for his/her careful modifications.

2. Some parts of the review seem to be a bit too long. For instance, the quantum optics implementation described in section 3.2 has been described by the people who did that work and by top experts on this as "the most expensive way to diagonalize a 2x2 matrix" and the text of the review should describe that work using those words inside the quotation marks, because these convey the reality of that paper, which has been oversold to the press. Indeed, that paper was rejected by several journals, before it was published, because it was ill-designed.

It takes a simple task (diagonalizing a 2x2), and transforms it into a massively messy one, with complex optics and also classical computers helping the process. It is surprising that section 3.2 would devote so much space to "the most expensive way to diagonalize a 2x2 matrix".

Ans: We have modified this part in section 3.2, especially some sentences which might be oversold to the press. For example, we have changed "Despite the other steps of the algorithm are assisted by a classical computer, the key step of performing the iterative PEA is realized perfectly on a linear optical quantum system, yielding important progress towards simulating quantum chemistry." to "The key step of performing the iterative PEA was realized on a linear optical quantum system, and the other steps of the algorithm including initial state preparation were assisted by a classical computer."

3. Section 4.2 also devotes too much space to ref. 60, which is over-emphasized there. Namely, papers that have been oversold before, are still overrated here.

Ans: We conjectured that Referee 2 was aiming at section 4.1, as this section was dominated by ref. 60. We have changed some sentences which might be over-emphasized, and deleted the details of describing the Trotter-Suzuki formula to shorten this part.

4. The reference section could be more balanced. Now it is dominated by two groups: HU and USTC. Same with the text of the review: too much emphasis on works by these two groups, specially HU. Yes, these two groups have done considerable work in this area, but too much focus on two groups makes the review less appealing to a broader audience. Also, the excellent USTC work has not been oversold to the press, in my opinion, but the one from HU has been, according to many. Different (boasting) styles.

Ans: We have added some sentences and more than ten references of other groups to make this manuscript more balanced. For example, in section 1.3, we added two references (T. Ladd et al., Nature, 2010, 464, 45 and I. Buluta et al., Rep. Prog. Phys., 2011, 74, 104401) which review the recent progress in the physical realization of quantum simulation, and some work in superconducting circuits. In the end of section 4.1, we added one paragragh including two references (A. Smirnov et al., Eur. Phys. Lett., 2007, 80, 67008 and E. Torrontegui et al., J. Phys. B: At. Mol. Opt. Phys., 2011, 44, 195302) of describing two AQS proposals about simulating chemical reactions. In the end of the last second paragraph of section 5, we mentioned one work about simulating the energy spectrum of the water molecule (H. Wang et al., 2011, arXiv:quant-ph/1108.5902v1).

5. For instance, the figures in the paper do not have references, and these are often indicated (in the best reviews) as "This figure is reproduced from ref. X", so the

reader of each caption would immediately know where the figures are taken from.

Ans: We added “Reproduced from Ref. XXX” in the captions of the relevant figures.

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List of Changes:
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1. We have nearly accepted all the modifications indicated in the attached document, and made some other minor corrections in grammar.
2. We have added one leading sentence and two review references to guide the following description of feasible physical systems for quantum simulation in section 1.3.
3. We have added some references in the part of introducing superconducting circuits in section 1.3.
4. We have rewritten 2.2.2 in detail to make it comprehensible for non-specialists.
5. We have modified some sentences which may be oversold to the press in the part of introducing the quantum linear optical experiment in section 3.2.
6. We have deleted and rewritten some sentences in section 4.1 to avoid it too long and over-emphasized.
7. We have added one paragraph to introduce two AQS proposals of simulating chemical reactions.
8. We have added one work about simulating the energy spectrum of the water molecule in the last second paragraph of section 5.
9. We have added underlines in Fig. 3 to show the experimental results clearly.
10. We have changed the unit “Angstrom” to “\AA” in Fig. 4(b).
11. We have stated where the figures are taken from in the caption of the figures by “Reproduced from Ref. XXX.”

We sincerely hope that the revised version is now acceptable for publication in Physical Chemistry Chemical Physics.

Thank you for your kind attention.
Sincerely,
Dr. Jiangfeng Du
Professor of Physics