TO: Dr. Claudia Pate

Physical Review Letters

Dear Dr. Claudia Pate,

Thank you for sending the PDF proof of our manuscript LE13229. The following is our corrections to the proof.

Since the proof has 5 pages (exceeding about 10 lines), we made the modifications (a)-(h) to save the necessary space. The deleted text is not very necessary in understanding this paper. The meaning of the text is not weakened and our previous revisions due to referees’ comments are all kept. If possible, we would also like to have a second proof when the following changes are implemented.

1. In the last paragraph of the “Introduction” part, please delete the sentence “To our knowledge, this is the first explicit implementation of the quantum simulation of a chemical reaction process.”. It is fate to do so because we already said this in the first paragraph. This saves 2 lines.
2. In the “Theory” section, please delete the beginning 1.5 sentences, i.e., “Previously we were able to simulate the ground-state energy of a hydrogen molecule [18]. Here,” and then change “to” to “To”. This saves 1 line.
3. Under Eq. (4), please delete “, including an error analysis of the split-operator technique,” This saves 1 line.
4. Under Eq. (7), please delete the sentence “Such a loop of operations is m-dependent because the simulated system is subject to a time-dependent laser field.” This saves 2 lines.
5. In the “Conclusion” section, please delete “A quantum simulator attacking problems not solvable on current classical computers will be one conceivable milestone in the very near future. The realization of” and then change “quantum simulations…” to “Quantum simulations…”. That is, “Quantum simulations” are now the start of the first sentence of the conclusion section. This saves 2 lines.
6. In the “Conclusion” section, please change the sentence “Our work reported here is the first experimental study of the quantum simulation of a prototype laser-driven chemical reaction. This is made possible by” to “Our simulation of a prototype chemical reaction is made possible by”. This rephrasing saves 2 lines.
7. In the caption of Fig.2a, please change the sentence “Diagonal elements are the Larmor frequencies (Hz), and off diagonal elements are scalar coupling strength (Hz) between two nuclear spins. Relaxation and dephasing time scales (second) T1 and T2 for each nuclear spin are listed on the right.” to “The Larmor frequencies (Hz), the scalar coupling strength (Hz), the relaxation and dephasing time scales (second) T1 and T2 are listed in the table.” This saves 1 line.
8. In the caption of Fig. 3(a),(b): please delete “based on an eight-dimensional Hilbert space”. This saves 1 line.

The total number of saved lines is about 11~12 lines. We hope that the length of the paper is compressed into exactly 4 pages now.

Here are the answers to the questions and comments.

1. The added “Singapore” is fine.
2. Yes, the conference was held in Santa Fe as shown.
3. We checked the external links and found them all correct.
4. The changes to Ref. [6] are fine.
5. For the brief description of the supplemental material, please use the phrase “for technical and experimental details”.
6. The reference [29] can be found at <http://www.cap.ca/en/article/quantum-information-processing-using-nuclear-and-electron-magnetic-resonance-review-and-pros>.
7. The changes about the fractions in superior mode are all right.
8. The new subscript “expt” is correct.
9. It is our mistake to have a redundant opening parenthesis. Please delete this redundant opening parenthesis in the radical.

Besides, “a NMR quantum simulator” in the paper title should be “an NMR quantum simulator” in our opinion.

Thank you for your kind attention.

Sincerely,

Dr. Jiangfeng Du

Professor of Physics