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April 9, 2022

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Dear Professor Yang,

Enclosed is our manuscript entitled, "**New Phase Space Formulations and Quantum Dynamics Approaches**", by Xin He, Baihua Wu, Youhao Shang, Binqi Li, Xiangsong Cheng, and myself, which we resubmit for publication in *WIREs Computational Molecular Science* as a Focus Article.

We describe below our replies to specific questions of the two referees, and our revisions in light of them.

Many thanks!

Yours sincerely

Jian Liu

Replies to Reviewers' Comments:

Reviewer #1

Comments to the Author(s):

In this paper, the authors have overviewed the recent progress on the phase space formulation of quantum mechanics with constraint coordinate-momentum variables for discrete variable quantum systems. Various numerical tests in gas phases and condensed phases have shown that the new trajectory-based quantum dynamics approaches with this phase space representation are useful and practical for describing processes of composite quantum systems. The topic is important and paper is acceptable for publication after following revision.

1) Because all rigorous phase space representations are one-to-one correspondence mapping, it will be interesting to show the relation or transformation between (weighted) CPS and the Stratonovich phase space for finite-variable systems, similarly, that between Wigner and Husimi representations for continuous-variable systems.

Reply: We have followed the reviewer's suggestion to add the content. The relation between CPS and Stratonovich phase space is discussed in detail in Appendix 3. The relation between Wigner and Husimi representations is added at the end of Section 2.1. (Changes are marked in red.)

2) It will be more useful to expand Appendix 2 for both constraint phase space (CPS) as well as weighted CPS. Because this part is essential to understand the most important theory in the article, more details will help others follow the derivation.

Reply: Done. We have expanded the derivation of CPS and weighted CPS in Appendix 1. (Changes are marked in red.)

3) Most references include the full journal name, but several references use the abbreviation of the journal. It should be consistent.

Reply: Done. The format of all references has been unified.

Reviewer #2

Comments to the Author(s):

This is an interesting and well-written paper that focuses on recent advances in the authors' phase space approach to quantum dynamics. The is work falls in the general area of "mapping" approaches to treating the quantum degrees of freedom in mixed quantum-classical dynamics, which is one of the most important and active areas currently in theoretical chemistry. Liu and his coworkers are leaders in this field, and their work in this field is characterized by rigor and clarity, which has made an important contribution to addressing the significant fundamental and practical challenges of this approach. The current focus adds to this body of work. Here, they focus on their weighted constraint coordinate-momentum phase space formulation. This new approach is described and compared with previous methods in a number of careful studies. This is a broad field, the authors do a good job of recognizing and summarizing the work of others while focusing on their own contributions. The paper is succinct but clear and complete, and is a good introduction to this significant and fascinating field. This paper will be of high interest to the readers of the journal, and appears to be scientifically correct. The paper is quite suitable for publication in its present form.

Reply: We appreciate the comments of the referee.