

WIREs Computational Molecular Science

Decision Letter (CMS-842)

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Subject: Decision on Manuscript ID CMS-842

Body: Dear Dr. Liu,

I am writing in regards to Manuscript ID CMS-842 entitled "New Phase Space Formulations and Quantum Dynamics Approaches," which you submitted to WIREs Computational Molecular Science. The reviewer(s) have recommended publication, but also suggest some minor revisions. Their comments are included at the bottom of this letter; I invite you to respond to them and revise your manuscript.

Please submit your revision within 3 weeks. If you need extra time, please let us know so that we can keep our systems updated for editorial planning purposes.

A revised version of your manuscript that takes into account the comments of the reviewer(s) will be reconsidered for publication.

If you are updating your Main Document in Word, make sure that "Track Changes" is enabled so that the editors can easily find your amendments. If you are using LaTeX, make sure that revisions are made in red font.

You can upload your revised manuscript using this direct link: *** PLEASE NOTE: This is a two-step process. After clicking on the link, you will be directed to a webpage to confirm. ***

https://mc.manuscriptcentral.com/compmolsci?URL_MASK=830e909372ac4be195c372815e653813.

When you submit your revision, you must provide a point-by-point summary of how each of the issues raised by the reviewer(s) were addressed. Please note that the space provided is for plain text only, as the system will not accept any formatting. For each criticism raised, please provide:

1. The criticism from the reviewer.
2. The response and explanation of how the manuscript has been modified in response to the criticism.

IMPORTANT: We have your original files; therefore, please delete the file(s) that you wish to replace and then upload the revised file(s). You will be able to upload both marked and clean versions of your Main Document. Please note that figures must be in PRODUCTION-READY format.

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Please do not hesitate to get in touch with us if you have any queries or concerns.

Once again, thank you for submitting your article to WIREs Computational Molecular Science. I look forward to receiving your revision.

Sincerely,

Prof. Jinlong Yang
Editor, WIREs Computational Molecular Science
jlyang@ustc.edu.cn

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

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 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.

Date Sent: 15-Mar-2022

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