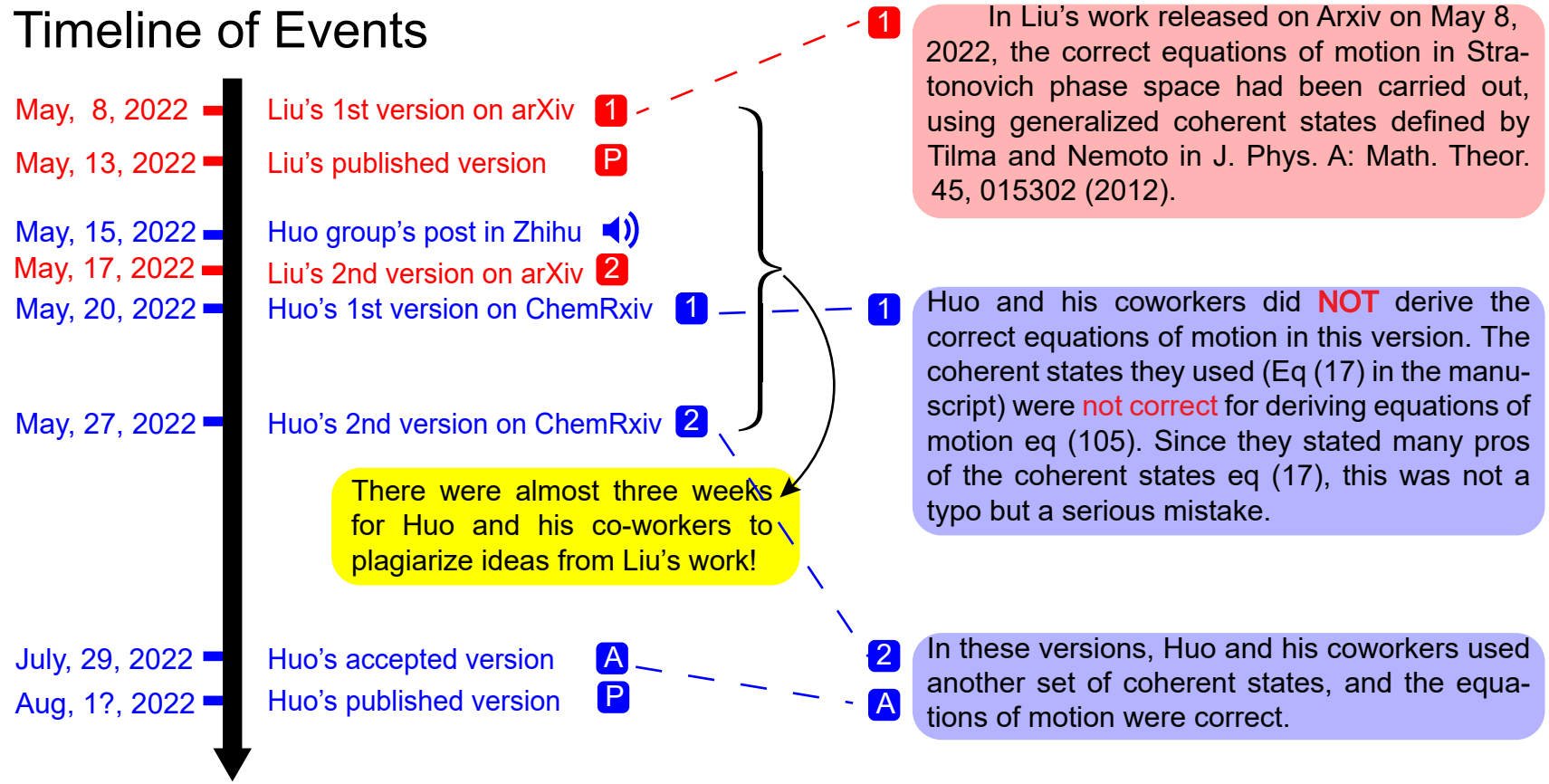
Timeline of Events



1 https://arxiv.org/abs/2205.03870v1

P https://doi.org/10.1002/wcms.1619

2 https://arxiv.org/abs/2205.03870v2

https://www.zhihu.com/people/liu-xing-yu-72-53/pins

1 https://chemrxiv.org/engage/chemrxiv/article-details/6286c9ba59f0d6831996a480

2 https://chemrxiv.org/engage/chemrxiv/article-details/6290092c1df2edd1ac59ea52

A https://aip.scitation.org/doi/10.1063/5.0094893

P https://aip.scitation.org/doi/10.1063/5.0094893

Evidence 3: FATAL MISTAKE

Evidence #3:

In Version 1 of Huo and his coworkers(first released online to ChemRxiv on **May 20, 2022**), the equations of motion eqs (98), (101) and (105), **with the coherent states eq (17),** were actually **wrong**. The authors even **emphasized** the various pros of their new spin coherent states. It means that the inconsistence was not because of typos, but serious mistakes.

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where the expansion coefficients are

$$\langle n|\mathbf{\Omega}\rangle = \begin{cases} \cos\frac{\theta_1}{2}e^{-i\frac{\varphi_1}{2}} & n=1, \\ \cos\frac{\theta_n}{2}e^{-i\frac{\varphi_n}{2}}\prod_{l=1}^{n-1}\sin\frac{\theta_l}{2}e^{i\frac{\varphi_l}{2}} & 1<n<N, \\ \prod_{l=1}^{N-1}\sin\frac{\theta_l}{2}e^{i\frac{\varphi_l}{2}} & n=N. \end{cases} \tag{17}$$

with $\{\theta_n\} \in [0,\pi]$ and $\{\varphi_n\} \in [0,2\pi]$. The expansion coefficients can be derived from the usual recursive expression[29] given in Eq. B1. Note that the definition of the spin-coherent states used here is different than those used in the previous generalized spin mapping formalism[29] as we symmetrically split the phase $e^{i\varphi_n}$ between $|n\rangle$ and $|n+1\rangle$ states, which allows to conveniently transform all of these coefficients into the phase space mapping variables later (see Eq. 44). This is necessary in order to introduce both real and imaginary part of the expansion coefficient c_n (for all n) as the phase space mapping variables, which will be discussed in Sec. III D.

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The equations of motion were **incorrect** for systems with 3 or more electronic states, however *happened to be correct* for two-electronic-state systems. (See Numerical tests in ***)

Though they added a note, Ref. 56 in their Version 2 (first released online to ChemRxiv on **May 27, 2022**), stating that their mistakes did not affect physical expectations, it *truly* affects dynamics and can make severe problems in numerical tests(See Numerical tests in ***). It is then very suspicious that the results obtained by the authors for the three-state system in Figures 4 and 5 of Version 1 did not faithfully employ their **wrong** equations of motion. We must seriously query that whether the data were made-up? The authors should provide the original source code for Figure 4 and 5 of Version 1 to do the investigation.

In our paper *Wiley Interdiscip. Rev. Comput. Mol. Sci.* e1619 (2022) [submitted on **February 5, 2022**, released on arXiv on **May 8, 2022** and officially published on **May 13, 2022**], we had already published the correct EOMs on Stratonovich phase space before the online time of Huo *et al.*'s two Versions. It is evident that Huo and his coworkers carefully studied our arXiv preprint paper before **May 27, 2022** (see Evidence #?).

Nearly three weeks existed between **May 8, 2022** and **May 27, 2022**, which should have been enough for Huo and his coworkers to plagiarize the ideas of the correct EOMs in the *Wiley Interdiscip. Rev. Comput. Mol. Sci.* e1619 (2022) preprint/paper,

and then realized their EOMs were wrong. The plagiarism did take Huo and his coworkers quite some time. Although the Huo group claimed on **May 14, 2022 (Rochester Time)** that they had already been studying the arXiv preprint of *Wiley Interdiscip. Rev. Comput. Mol. Sci.* e1619 (2022) [submitted on **February 5, 2022**, released on **arXiv on May 8**, 2022 and officially published on **May 13, 2022**], they still failed to understand that their EOMs of Version 1 were wrong until at least **May 20, 2022**, when Version 1 was released on ChemRxiv. Not until **May 27, 2022** did Huo and his coworkers released their Version 2 that finally included the correct EOMs.

Table 1: Comparisons of Version 1 and Version 2

Version 1 (first released online to ChemRxiv on May 20, 2022)	**Version 2 (first released online to ChemRxiv on May 27, 2022)**
$\|\mathbf{u}\rangle = \cos\frac{\theta}{2}e^{-i\varphi/2}\|1\rangle + \sin\frac{\theta}{2}e^{i\varphi/2}\|2\rangle$ (15)	$\|\mathbf{u}\rangle = \cos\frac{\theta}{2}\|1\rangle + \sin\frac{\theta}{2}\cdot e^{i\varphi}\|2\rangle$ (16)
$\langle n\|\mathbf{\Omega}\rangle = \begin{cases} \cos\frac{\theta_1}{2}e^{-i\frac{\varphi_1}{2}} & n=1, \\ \cos\frac{\theta_n}{2}e^{-i\frac{\varphi_n}{2}}\prod_{l=1}^{n-1}\sin\frac{\theta_l}{2}e^{i\frac{\varphi_l}{2}} & 1<n<N, \\ \prod_{l=1}^{N-1}\sin\frac{\theta_l}{2}e^{i\frac{\varphi_l}{2}} & n=N. \end{cases}$ (17)	$\langle n\|\mathbf{\Omega}\rangle = \begin{cases} \cos\frac{\theta_1}{2} & n=1, \\ \cos\frac{\theta_n}{2}\prod_{l=1}^{n-1}\sin\frac{\theta_l}{2}e^{i\varphi_l} & 1<n<N, \\ \prod_{l=1}^{N-1}\sin\frac{\theta_l}{2}e^{i\varphi_l} & n=N. \end{cases}$ (18)
No corresponding part	[56]Note that the usual way to write down this state is $\|\mathbf{u}\rangle = \cos\frac{\theta}{2}e^{-i\varphi/2}\|1\rangle + \sin\frac{\theta}{2}\cdot e^{i\varphi/2}\|2\rangle$. This specific choice of splitting phase φ does not influence any physical expectation values we aim to calculate.

Table 2: Comparisons of Version 1 and Version 3

Version 1 (first released online to ChemRxiv on May 20, 2022)	**Version 3 (accepted online on July 29, 2022)**
$\|\mathbf{u}\rangle = \cos\frac{\theta}{2}e^{-i\varphi/2}\|1\rangle + \sin\frac{\theta}{2}e^{i\varphi/2}\|2\rangle$ (15)	$\|\mathbf{u}\rangle = \cos\frac{\theta}{2}\|1\rangle + \sin\frac{\theta}{2}\cdot e^{i\varphi}\|2\rangle$ (16)
$\langle n\|\mathbf{\Omega}\rangle = \begin{cases} \cos\frac{\theta_1}{2}e^{-i\frac{\varphi_1}{2}} & n=1, \\ \cos\frac{\theta_n}{2}e^{-i\frac{\varphi_n}{2}}\prod_{l=1}^{n-1}\sin\frac{\theta_l}{2}e^{i\frac{\varphi_l}{2}} & 1<n<N, \\ \prod_{l=1}^{N-1}\sin\frac{\theta_l}{2}e^{i\frac{\varphi_l}{2}} & n=N. \end{cases}$ (17)	$\langle n\|\mathbf{\Omega}\rangle = \begin{cases} \cos\frac{\theta_1}{2} & n=1, \\ \cos\frac{\theta_n}{2}\prod_{l=1}^{n-1}\sin\frac{\theta_l}{2}e^{i\varphi_l} & 1<n<N, \\ \prod_{l=1}^{N-1}\sin\frac{\theta_l}{2}e^{i\varphi_l} & n=N. \end{cases}$ (18)