Evidence 2: PLAGIARISM

Timeline of Events

- July 9, 2019 — Liu's J. Chem. Phys. 151, 024105 (2019) published online
- March 5, 2021 — Liu's J. Phys. Chem. Lett. 12, 2496 (2021) published online
- August 2, 2021 — Liu's J. Phys. Chem. A 125, 6845 (2021) published online
- November 10, 2021 — Liu's Acc. Chem. Res. 54, 4215 (2021) published online
- May 8, 2022 — Liu's 1st version on arXiv 1
- May 13, 2022 — Liu's published version P
- May 15, 2022 — Huo group's post on Zhihu
- May 17, 2022 — Liu's 2nd version on arXiv 2
- May 20, 2022 — Huo's 1st version on ChemRxiv 1
- May 27, 2022 — Huo's 2nd version on ChemRxiv 2
- July, 29, 2022 — Huo's accepted version A
- Aug, 1?, 2022 — Huo's published version P

There were almost three weeks for Huo and his co-workers to plagiarize ideas from Liu's work!

Statements

In this paper, we first pointed out that the sum of the electron populations is equal to 1 is a natural constraint for the Meyer-Miller mapping variables for general *F*-state systems, when parameter γ=0:

$$\sum_{n=1}^{F}\frac{1}{2}\left[\left(x^{(n)}\right)^2+\left(p^{(n)}\right)^2\right]=1$$

In these papers, we further extended the relations to any γ>-1/F for general *F*-state systems:

$$\sum_{n=1}^{F}\frac{1}{2}\left[\left(x^{(n)}\right)^2+\left(p^{(n)}\right)^2\right]=1+F\gamma$$

Plagiarized from

The constraint of the Meyer-Miller mapping variables:

$$\sum_{n=1}^{N}\frac{1}{2}\left(p_n^2+q_n^2-\gamma\right)=1$$

Evidence #2:

In the last paragraph of page 7 of Version 1 of Huo and his coworkers(first released online to ChemRxiv on **May 20, 2022**):

"

In the $\mathfrak{su}(N)$ mapping formalism, the total population constraint on the $2N$-dimensional phase space comes naturally from the normalization of the generalized spin coherent state[53,57] as follows

$$\langle \mathbf{\Omega} | \mathbf{\Omega} \rangle = \sum_n c_n^* c_n = \frac{1}{2r_s} \sum_{n=1}^{N} (q_n^2 + p_n^2) = 1, \qquad (53)$$

which properly enforces the total electronic diabatic population to be one for these MMST mapping variables

$$\boxed{\sum_{n=1}^{N} \frac{1}{2}(q_n^2 + p_n^2 - \gamma) = 1.} \qquad (54)$$

Alternatively, one can obtain this condition from the basic property of the SW transform that preserves the trace of the electronic identity operator (Eq. 28) as follows

$$[\hat{\mathcal{I}}]_s = \sum_{n=1}^{N} [|n\rangle\langle n|]_s = 1 - r_s + \sum_n \frac{1}{2}(q_n^2 + p_n^2) = 1.$$

"

as well as the lower left part of page 9 of Version 2 (first released online to ChemRxiv on **May 27, 2022**):

"

In the $SU(N)$ mapping formalism, the total population constraint on the $2N$-dimensional phase space comes *naturally* from the normalization of the generalized spin coherent states[69,75] as follows

$$\langle \mathbf{\Omega} | \mathbf{\Omega} \rangle = \sum_n c_n^* c_n = \frac{1}{2r_s} \sum_{n=1}^{N} (q_n^2 + p_n^2) = 1, \qquad (56)$$

which properly enforces the total electronic diabatic population to be one (see Eq. 51) for these MMST mapping variables

$$\boxed{\sum_{n=1}^{N} \frac{1}{2}(q_n^2 + p_n^2 - \gamma) = 1.} \qquad (57)$$

Alternatively, one can obtain this condition from the basic property of the S-W transform that preserves the trace of the electronic identity operator (Eq. 30) as follows

$$\boxed{\left[\hat{\mathcal{I}}\right]_{\mathrm{s}} = \sum_{n=1}^{N} \left[|n\rangle\langle n|\right]_{\mathrm{s}} = 1 - r_{\mathrm{s}} + \sum_{n} \frac{1}{2}(q_n^2 + p_n^2) = 1.}$$

Note that the recent work of the eCMM is developed based on *manually* adding an extra total population constraint (as described in Eq. 57) on the MMST mapping oscillator phase space. Historically, it was realized[75] that a mapping from the quantum Schrödinger's equation to $2N$ classical phase space Hamilton's EOMs is incorrect,

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and the left part of page 24 of Version 3 (accepted on **July 29, 2022**):

"

In the $SU(N)$ mapping formalism, the total population constraint on the $2N$-dimensional phase space comes *naturally* from the normalization of the generalized spin coherent states[69,108] as follows

$$\langle \mathbf{\Omega}|\mathbf{\Omega}\rangle = \sum_{n} c_n^* c_n = \frac{1}{2r_{\mathrm{s}}} \sum_{n=1}^{N} (q_n^2 + p_n^2) = 1, \qquad \text{(D11)}$$

which properly enforces the total electronic diabatic population to be one (see Eq. D6) for these MMST mapping variables

$$\boxed{\sum_{n=1}^{N} \frac{1}{2}(q_n^2 + p_n^2 - \gamma) = 1. \qquad \text{(D12)}}$$

Alternatively, one can obtain this condition from the basic property of the S-W transform that preserves the trace of the electronic identity operator (Eq. 30) as follows

$$\boxed{\left[\hat{\mathcal{I}}\right]_{\mathrm{s}} = \sum_{n=1}^{N} \left[|n\rangle\langle n|\right]_{\mathrm{s}} = 1 - r_{\mathrm{s}} + \sum_{n} \frac{1}{2}(q_n^2 + p_n^2) = 1.}$$

Note that the recent work of the eCMM is developed based on *manually* adding an extra total population constraint (as described in Eq. D12) on the MMST mapping oscillator phase space. Historically, it was realized[108] that a mapping from the quantum Schrödinger's equation

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Huo and his coworkers mentioned the constraint that the sum over electronic population is equal to 1, but neglected the fact that this normalization/constraint had been first proposed in eq (28) of *J. Chem. Phys.* 151, 024105 (2019) [submitted on **May 1, 2019**, accepted on **June 11, 2019** and published on **July 9, 2019**]:

"

$\boxed{\text{The conservation of the total population}}$ Eq. (16) is implicitly used for the kinetic energy term in Eq. (23). (This is a new observation that is essentially the key point of this paper.) The classical Hamiltonian for both nuclear and electronic DOFs is then

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“

$$\boxed{\sum_{n=1}^{F} P_n(0) = 1} \text{ and } 0 \leq P_n(0) \leq 1 \quad (\forall n). \tag{28}$$

”

In the paper *J. Chem. Phys.* 151, 024105 (2019), the constraint phase space manifold had been firstly utilized by us to implement phase space mapping for nonadiabatic dynamics, which in principle could be parameterized by either Meyer-Miller variables or (Stratonovich) angle variables. Using this constraint, the Q, W, or P versions of Stratonovich phase space used in spin mapping methods proposed in *J. Chem. Phys.* 152, 084110 (2020) were only three special cases of the constraint coordinate-momentum phase space in classical mapping model(CMM) methods. Later, the relationship was further clarified again 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**]. Neither Version 1 nor Version 2 of Huo and his coworkers cited this article.

In our *J. Phys. Chem. Lett.* 12, 2496–2501 (2021) [submitted on **January 22, 2021**, accepted on **February 19, 2021** and published online on **March 5, 2021**], we had clearly clarified the one-to-one mapping (i.e., mapping and inversed mapping) between identity operator and 1:

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Supporting Information.) As expected, the kernel and its inverse are properly normalized

$$\boxed{\begin{gathered}\mathrm{Tr}_e[\hat{K}(\mathbf{x},\mathbf{p})] = \mathrm{Tr}_e[\hat{K}^{-1}(\mathbf{x},\mathbf{p})] = 1 \\ \int_{S(\mathbf{x},\mathbf{p})} \mathrm{d}\boldsymbol{\mu}(\mathbf{x},\mathbf{p})\,\hat{K}(\mathbf{x},\mathbf{p}) = \int_{S(\mathbf{x},\mathbf{p})} \mathrm{d}\boldsymbol{\mu}(\mathbf{x},\mathbf{p})\,\hat{K}^{-1}(\mathbf{x},\mathbf{p}) = \hat{I}_e \qquad (9)\end{gathered}}$$

where $\hat{I}_e$ is the identity operator in F-dimensional Hilbert space

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It is natural that the constraint of the manifold corresponds to the one-to-one mapping conditions, thus it is never a *“manually”* added constraint. Huo and his coworkers interpreted *our* ideas in **their** way and claimed **they** firstly got these ideas.