Evidence 5: PLAGIARISM

Timeline of Events

- 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!

[1] In Liu's work released on Arxiv on May 8, 2022, the term "smooth manifold" appeared in the introduction section, and was used to describe phase spaces, including groups. The term "diffeomorphic" appeared in Appendix 3, which was used to describe relationship between differentiable manifolds.

[1] Neither "smooth manifold" nor "differentiable manifold" appeared in Huo's first version even until May 20, 2022, and in this version groups were not described as manifolds.

[2] In this version, the term "differentiable manifold" first appeared, and Lie groups were described as manifolds; both these two kinds of changes were without citation.

[A] In this version, the term "smooth manifold" was directly copied from Liu's work without citation.

More than 10 places

[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 #5:

Huo and his coworkers directly copied our understanding on describing groups and phase spaces as smooth and differentiable manifolds.

The term, "smooth manifold", first appeared 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**], for describing phase spaces (including $SU(2)$ or $SU(F)$ *groups*):

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although a pure state was used for demonstration.[89] The most essential element is the one-to-one correspondence

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mapping between quantum operators and classical functions often defined on a smooth manifold, namely, phase space. Because of the commutation relation of conjugate operators, the mapping is not unique in quantum mechanics.[90,91]

Phase space representations of a finite discrete F-state quantum system were first independently described by Stratonovich[100] in 1956, Feynman[101] in 1987, and Wootters[102] in 1987. Further developments of Stratonovich's formulation have focused on an SU(2) or SU(F) structure of phase space,[103–117] while those on the construction of a discrete phase space are described in References 78,118–126. Other than the 2-state (or spin 1/2) system, the exact equations of motion

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and in our *Wiley Interdiscip. Rev. Comput. Mol. Sci.* e1619 (2022) the term "diffeomorphic" was used for describing differentiable manifolds (phase spaces) in Appendix 3:

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The second kind of representation is the SU(F) Stratonovich phase space. A kind as described by Tilma *et.al.* in ref [11] is diffeomorphic to the quotient set $\mathrm{SU}(F)/\mathrm{U}(F-1)$, parameterized by $(2F-2)$ angle variables $(\boldsymbol{\theta},\boldsymbol{\varphi}) = (\theta_1,\theta_2,\ldots,\theta_{F-1},\varphi_1,\varphi_2,\ldots,\varphi_{F-1})$. The range of each angle θ_i is

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Yet, neither "differentiable manifold" nor "smooth manifold" existed in Version 1 (first released online to ChemRxiv on **May 20, 2022**) of Huo and his coworkers, and groups were not described as manifolds. In Version 2 (first released online to ChemRxiv on **May 27, 2022**) of Huo and his coworkers, "differentiable manifold" and "Lie group/manifold" started to appear, and Huo and his coworkers started to describe groups as manifolds; and in Version 3 (accepted on **July, 29, 2022**) of Huo and his coworkers, the term "smooth manifold" were directly copied from ours. In not any of these cases were our works cited.

Such plagiarisms occurred in more than 10 places in Huo's revised version (Version 2/Version 3). An incomplete list of these kinds of plagiarism is shown below.

Table 1: Comparisons of Version 1 and Version 2

Version 1 (first released online to ChemRxiv on	**Version 2 (first released online to ChemRxiv on May**

May 20, 2022)	27, 2022)
(abstract) We present the rigorous theoretical framework of the generalized spin mapping representation for non-adiabatic dynamics. This formalism is based on the generators of the $\mathfrak{su}(N)$ Lie algebra to represent N discrete electronic states, thus preserving the size of the original Hilbert space in the state representation. We use the generalized spin coherent states representation and the Stratonovich-Weyl transform to describe these electronic spin-mapping variables in the $\boxed{\text{continuous variables space.}}$ Wigner representation is used to describe the nuclear degrees of freedom. Using the above representations, we derived an exact expression of the	**(abstract)** We present the rigorous theoretical framework of the generalized spin mapping representation for non-adiabatic dynamics. This formalism is based on the generators of the $\mathfrak{su}(N)$ Lie algebra to represent N discrete electronic states, thus preserving the size of the original Hilbert space in the state representation. The Stratonovich-Weyl trans~~form is then used to map an operator in the Hilbert space~~ to a continuous function on the $SU(N)$ Lie Group $\boxed{\textit{manifold} \text{ which is a phase space of continuous variables.}}$ Wigner representation is used to describe the nuclear degrees of freedom. Using the above representations, we derived an exact
(page 2) non-adiabatic dynamics in a N-state system. In particular, the Stratonovich-Weyl transform[30] is used to convert generalized spin operators (generators) into $\boxed{\text{continuous variables,}}$ resulting in a classical-like Hamiltonian that depends on $N^2 - 1$ expectation values of the spin operators under the generalized spin coherent states.[31,32] The spin coherent states are further expressed as a linear ex-	**(page 2)** Linearized semi-classical (spin-LSC) approach.[43] In particular, the Stratonovich-Weyl (S-W) transform[27,28,44,45] is used to map an operator in the Hilbert space described by the generators (of the $\mathfrak{su}(N)$ Lie algebra) to a continuous function on the $\boxed{\text{Lie group/manifold,}}$ resulting in a classical-like Hamiltonian. The S-W transform evaluates the expectation values of the spin operators under the generalized spin coherent states.[46,47] The gen-
(page 4) **III. STRATONOVICH-WEYL TRANSFORM OF THE $\mathfrak{su}(N)$ GENERATORS AND THE MAPPING FORMALISM** The *Stratonovich-Weyl* (SW) transform[30] can be used to evaluate the quantum electronic trace of an operator. Here, we present the properties of this transformation for a general N-level system.	**(page 5)** **III. STRATONOVICH-WEYL TRANSFORM AND THE SPIN MAPPING FORMALISM** The S-W transform constructs a mapping between an operator in the Hilbert space to a continuous function on the $\boxed{\text{Lie group/manifold.}}$ Here, we present the properties of this transformation for a general N-level system.
(page 5) Thus, Eq. 23 performs a mapping of an operator in the electronic subspace onto a phase space of continuous variables $\mathbf{\Omega}$ as follows $$\hat{A} \to [\hat{A}]_s(\mathbf{\Omega}). \quad (29)$$	**(page 6)** The S-W transform in Eq. 25 constructs a mapping between an operator in the Hilbert space to a continuous function whose variables are $\{\boldsymbol{\theta}, \boldsymbol{\varphi}\}$ or $\{\mathbf{\Omega}\}$ on the $\boxed{\text{Lie group/manifold.}}$ More specifically, this mapping relation is expressed as $$\hat{A} \longrightarrow [\hat{A}]_s(\mathbf{\Omega}), \quad (29)$$
No corresponding part	**(page 2)** Mathematically, the idea of mapping relation is referred to as the generalized Weyl correspondence, in which Lie groups and Lie algebras are the central components.[26–28] Lie algebras are formed by commutation relations among generators with given structure constants; the elements of a connected matrix Lie group[29] can be expressed as the exponential of the Lie algebra generators, *i.e.*, the exponential map.[30] On the other hand, a Lie group is also a $\boxed{\text{differentiable manifold,}}$ which is a $\boxed{\text{phase space}}$ with continuous variables. The dual identity of Lie groups naturally construct a bijective map between operators described by the generators represented in the Hilbert space and continuous functions on the $\boxed{\text{differentiable manifold}}$

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)

(abstract) We present the rigorous theoretical framework of the generalized spin mapping representation for non-adiabatic dynamics. This formalism is based on the generators of the $\mathfrak{su}(N)$ Lie algebra to represent N discrete electronic states, thus preserving the size of the original Hilbert space in the state representation. We use the generalized spin coherent states representation and the Stratonovich-Weyl transform to describe these electronic spin-mapping variables in the continuous variables space. Wigner representation is used to describe the nuclear degrees of freedom. Using the above representations, we derived an exact expression of the	**(abstract)** We present the rigorous theoretical framework of the generalized spin mapping representation for non-adiabatic dynamics. Our work is based up a new mapping formalism recently introduced by Runeson and Richardson in [J. Chem. Phys. 152, 084110 (2020)], which uses the generators of the $\mathfrak{su}(N)$ Lie algebra to represent N discrete electronic states, thus preserving the size of the original Hilbert space. Following this interesting idea, the Stratonovich-Weyl transform is used to map an operator in the Hilbert space to a continuous function on the $SU(N)$ Lie group, *i.e.*, a smooth *manifold* which is a phase space of continuous variables. We further use the Wigner representation to describe the nuclear degrees of freedom, and derived an exact expression of the time-correlation function as well as the exact quantum Liouvillian for
(page 2) non-adiabatic dynamics in a N-state system. In particular, the Stratonovich-Weyl transform[30] is used to convert generalized spin operators (generators) into continuous variables, resulting in a classical-like Hamiltonian that depends on N^2-1 expectation values of the spin operators under the generalized spin coherent states.[31,32] The spin coherent states are further expressed as a linear ex-	**(page 2)** Linearized semi-classical (spin-LSC) approach.[46] In particular, the Stratonovich-Weyl (S-W) transform[27,28,47,48] is used to map an operator in the Hilbert space described by the generators (of the $\mathfrak{su}(N)$ Lie algebra) to a continuous function on the Lie group/manifold, resulting in a classical-like Hamiltonian. The S-W transform evaluates the expectation values of the spin operators under
(page 4) **III. STRATONOVICH-WEYL TRANSFORM OF THE $\mathfrak{su}(N)$ GENERATORS AND THE MAPPING FORMALISM** The *Stratonovich-Weyl* (SW) transform[30] can be used to evaluate the quantum electronic trace of an operator. Here, we present the properties of this transformation for a general N-level system.	**(page 5)** **III. STRATONOVICH-WEYL TRANSFORM AND THE SPIN MAPPING FORMALISM** The S-W transform constructs a mapping between an operator in the Hilbert space and a continuous function on the Lie group/manifold. Here, we present the properties of this transformation for a general N-level system. Part of it has been previously discussed in the previous work by Runeson and Richardson.[35,46] To better help understanding the $SU(N)$ mapping formalism, we also provide the corresponding equations for the two-level system special case ($N=2$) in Appendix F.
(page 5) Thus, Eq. 23 performs a mapping of an operator in the electronic subspace onto a phase space of continuous variables $\mathbf{\Omega}$ as follows $\hat{A} \rightarrow [\hat{A}]_s(\mathbf{\Omega}). \quad (29)$	**(page 6-7)** where we have used the fact that $\int d\mathbf{\Omega} = N$ and Eq. 20. The S-W transform in Eq. 25 constructs a mapping between an operator in the Hilbert space to a continuous function whose variables are $\{\boldsymbol{\theta}, \boldsymbol{\varphi}\}$ or $\{\mathbf{\Omega}\}$ on the Lie group/manifold. More specifically, this mapping relation is expressed as $\hat{A} \longrightarrow [\hat{A}]_s(\mathbf{\Omega}), \quad (29)$
No corresponding part	**(page 2)**

	Mathematically, the idea of mapping relation is referred to as the generalized Weyl correspondence, in which Lie groups and Lie algebras are the central components.[26–28] Lie algebras are formed by commutation relations among generators with given structure constants; the elements of a connected matrix Lie group[29] can be expressed as the exponential of the Lie algebra generators, *i.e.*, the exponential map.[30] On the other hand, a Lie group is also a smooth manifold, which is a phase space with continuous variables. The dual identity of Lie groups naturally construct a bijective map between operators described by the generators represented in the Hilbert space and continuous functions on the differentiable manifold.