# Evidence 9: DATA FRAUD

## 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]

Figures in different versions (generated by different algorithms) were **totally the same**! It is almost impossible for Monte-Carlo based methods to show this kind of behavior.
We must propose that this is a serious **DATA FRAUD** event.

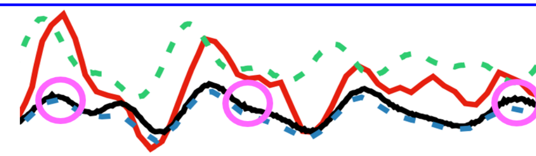
**Huo and his coworkers explained their EOMs of Stratonovich angle variables [eq(105) and eq(115)] in simulation details section.**

**Huo and his coworkers explained their EOMs of action-angle variables [eq(128) and eq(104)] in simulation details section.**

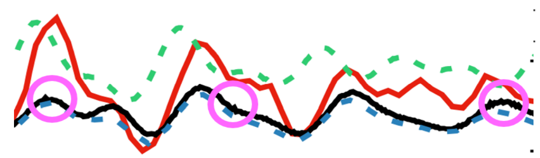
**Huo and his coworkers explained their EOMs of action-angle variables [eq(106) and eq(C8)] in simulation details section.**

For Example

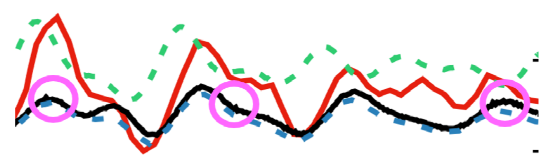
1 Fig. 3 lower panel



2 Fig. 3 lower panel



A Fig. 3 lower panel



[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 #9**

Here we report a suspect **data fraud** behavior of Huo and his coworkers. The figures in three versions of their manuscripts are **HIGHLY SIMILAR**. Due to the nature of Monte Carlo algorithm, these results **should not** be exactly the same, especially regarding that Huo and his coworkers claimed that the corresponding algorithms were **different**. This fact indicates high possibility of **DATA FRAUD**. The corresponding codes used to generate these figures must be provided by Huo and his coworkers.

**Table 1: Comparisons of Figure 3 of Version 1 and Version 2**

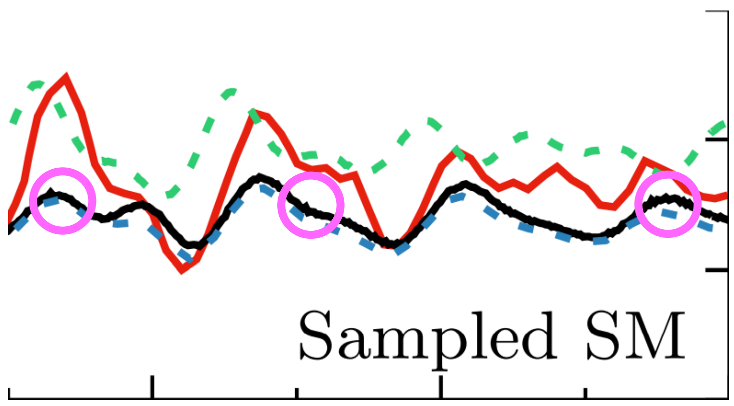
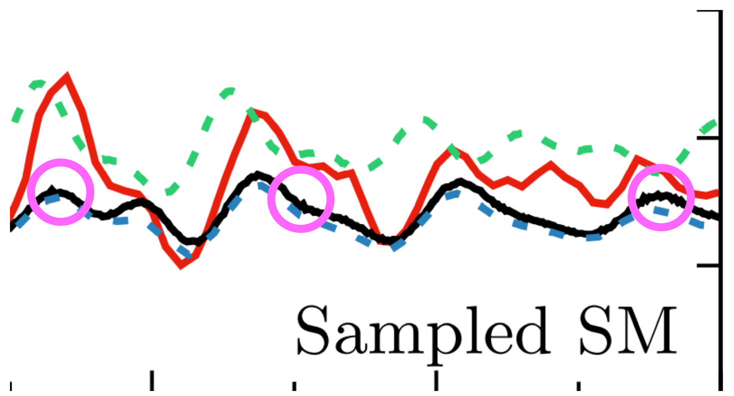
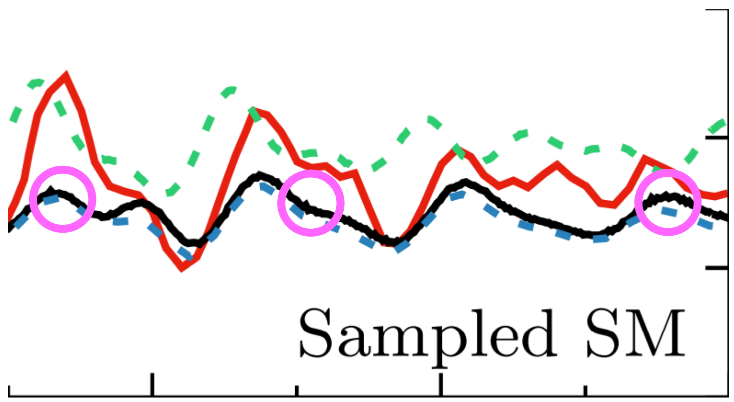
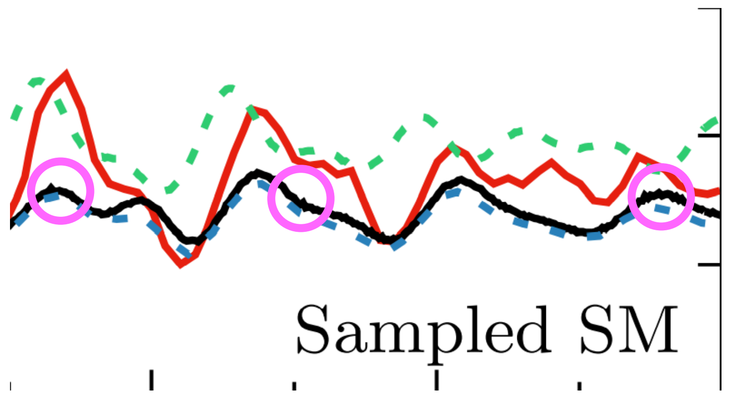
| From Version 1 (first released online to ChemRxiv on May 20, 2022), Fig. 3 (similarities circled by violet line) | From Version 2 (first released online to ChemRxiv on July 29, 2022), Fig. 3 (similarities circled by violet line) |
| --- | --- |
|   |   |

**Table 2: Comparisons of Figure 3 of Version 1 and Version 3**

| Version 1 (first released online to ChemRxiv on May 20, 2022), Fig. 3 (similarities circled by violet line) | Version 3 (accepted online on July 29, 2022), Fig. 3 (similarities circled by violet line) |
| --- | --- |
|   |   |

Huo and his coworkers had indicated in Version 1 and 2 that they used the EOMs on the Stratonovich phase space in numerical simulations:

**Table 3: Details of Version 1 and Version 2**

| From Version 1 (first released online to ChemRxiv on May 20, 2022) | From Version 2 (first released online to ChemRxiv on July 29, 2022) |
| --- | --- |

<table>
<tr>
<td>

## VI. MODEL SYSTEMS AND SIMULATION DETAILS

**Computational Method.** Using the EOMs expressed in Eq. 105 and the out-of-equilibrium TCF expressions that we derived in Eq. 71, we use the spin mapping approach under the linearized approximation to study the non-adiabatic dynamics of model systems.

are described in Eq. 77 and the procedure in Sec. IV. To propagate the dynamics, we use the simple Verlet algorithm because of the conjugate relation between $\Theta_n$ and $\varphi_n$ (see Eq. 98), as well as the relation between $\dot{\Theta}_n$ and $\dot{\theta}_n$ in Eq. 98a.

Different numerical algorithms!

First, the generalized angle variables $\{\varphi_n, \theta_n\}$ are propagated by a half time-step, which is done using the Verlet algorithm as follows

$$\theta_n(t+\frac{\Delta t}{4}) = \theta_n(t) + \dot{\theta}_n(t)\frac{\Delta t}{4}, \quad (115a)$$

$$\varphi_n(t+\frac{\Delta t}{2}) = \varphi_n(t) + \dot{\varphi}_n(t+\frac{\Delta t}{4})\frac{\Delta t}{2}, \quad (115b)$$

$$\theta_n(t+\frac{\Delta t}{2}) = \theta_n(t+\frac{\Delta t}{4}) + \dot{\theta}_n(t+\frac{\Delta t}{2})\frac{\Delta t}{4}, \quad (115c)$$

where $\dot{\theta}_n$ is expressed in Eq. 105c and $\dot{\varphi}_n$ is expressed in Eq. 105d. In theory it is possible to have a singular value

$$\dot{R} = \frac{P}{m}, \quad (105a)$$

$$\dot{P} = -\frac{\partial \mathcal{H}_0}{\partial R} - r_s \sum_{k=1}^{N^2-1} \frac{\partial \mathcal{H}_k}{\partial R}\Omega_k = -\frac{\partial H_s(R,P)}{\partial R}, \quad (105b)$$

$$\dot{\theta}_n = \Big(\frac{\partial H_s}{\partial \varphi_n}\frac{2}{\sin\theta_n} - \frac{\partial H_s}{\partial \varphi_{n-1}}\tan\frac{\theta_n}{2}\Big)\Big/\Big(r_s\prod_{j=1}^{n-1}\sin^2\frac{\theta_j}{2}\Big), \quad (105c)$$

$$\dot{\varphi}_n = \frac{\dot{\Omega}_{\beta_{n+1,n}}\Omega_{\alpha_{n+1,n}} - \Omega_{\beta_{n+1,n}}\dot{\Omega}_{\alpha_{n+1,n}}}{\Omega^2_{\alpha_{n+1,n}} + \Omega^2_{\beta_{n+1,n}}}. \quad (105d)$$

</td>
<td>

## VII. SIMULATION DETAILS

Here, we document the computational method as well as the initial conditions. Details of the model systems are provided in Appendix G.

**Computational Method.** Using the EOMs expressed in Eq. 113 or Eq. 104 and the out-of-equilibrium TCF expressions that we derived in Eq. 73, we use the spin mapping approach under the linearized approximation to study the non-adiabatic dynamics of model systems. Here, we briefly summarize the details of the prop-

To propagate the dynamics, we use the simple Verlet algorithm because of the conjugate relation between $\Theta_n$ and $\varphi_n$ (see Eq. 109), as well as the relation between $\dot{\Theta}_n$ and $\dot{\theta}_n$ in Eq. 109a (to use the EOMs in Eq. 113).

First, the generalized conjugate variables $\{\varphi_n, \Theta_n\}$ are propagated by a half time-step, which is done using the Verlet algorithm as follows

$$\Theta_n(t+\frac{\Delta t}{4}) = \Theta_n(t) + \dot{\Theta}_n(t)\frac{\Delta t}{4}, \quad (128a)$$

$$\varphi_n(t+\frac{\Delta t}{2}) = \varphi_n(t) + \dot{\varphi}_n(t+\frac{\Delta t}{4})\frac{\Delta t}{2}, \quad (128b)$$

$$\Theta_n(t+\frac{\Delta t}{2}) = \Theta_n(t+\frac{\Delta t}{4}) + \dot{\Theta}_n(t+\frac{\Delta t}{2})\frac{\Delta t}{4}, \quad (128c)$$

or equivalently with $\theta_n$ instead of $\Theta_n$, where $\dot{\theta}_n$ and $\dot{\varphi}_n$ are expressed in Eq. 113a-113b and $\dot{\Theta}_n$ and $\dot{\varphi}_n$ in Eq. 104a-104b. In theory it is possible to have a singu-

$$\dot{\theta}_n = \Big(\frac{\partial H_s}{\partial \varphi_n}\frac{2}{\sin\theta_n} - \frac{\partial H_s}{\partial \varphi_{n-1}}\tan\frac{\theta_n}{2}\Big)\Big/\Big(r_s\prod_{j=1}^{n-1}\sin^2\frac{\theta_j}{2}\Big), \quad (113a)$$

$$\dot{\varphi}_n = \frac{\dot{\Omega}_{\beta_{n+1,n}}\Omega_{\alpha_{n+1,n}} - \Omega_{\beta_{n+1,n}}\dot{\Omega}_{\alpha_{n+1,n}}}{\Omega^2_{\alpha_{n+1,n}} + \Omega^2_{\beta_{n+1,n}}}, \quad (113b)$$

</td>
</tr>
</table>

**Table 4: Details of Version 1 and Version 3**

<table>
<tr>
<th>Version 1 (first released online to ChemRxiv on May 20, 2022)</th>
<th>Version 3 (accepted online on July 29, 2022)</th>
</tr>
<tr>
<td>

## VI. MODEL SYSTEMS AND SIMULATION DETAILS

**Computational Method.** Using the EOMs expressed in Eq. 105 and the out-of-equilibrium TCF expressions that we derived in Eq. 71, we use the spin mapping approach under the linearized approximation to study the non-adiabatic dynamics of model systems.

</td>
<td>

## VII. COMPUTATIONAL DETAILS

Here, we provide the computational implementation of the method. Details of the model systems, as well as the initial conditions of the simulations are provided in Supplementary Material Sec. VII.

Using the EOMs expressed in Eq. 86 or Eq. C8, and the out-of-equilibrium TCF expressions that we derived in Eq. 60, we can apply the linearized spin mapping approach to study the non-adiabatic dynamics of model systems. Here, we briefly summarize the details of the prop-

</td>
</tr>
</table>

| | |
|---|---|
| are described in Eq. 77 and the procedure in Sec. IV. To propagate the dynamics, we use the simple Verlet algorithm because of the conjugate relation between $\Theta_n$ and $\varphi_n$ (see Eq. 98), as well as the relation between $\dot{\Theta}_n$ and $\dot{\theta}_n$ in Eq. 98a. Different numerical algorithms!<br><br>First, the generalized angle variables $\{\varphi_n, \theta_n\}$ are propagated by a half time-step, which is done using the Verlet algorithm as follows<br><br>$\theta_n(t+\frac{\Delta t}{4}) = \theta_n(t) + \dot{\theta}_n(t)\frac{\Delta t}{4}$, (115a)<br>$\varphi_n(t+\frac{\Delta t}{2}) = \varphi_n(t) + \dot{\varphi}_n(t+\frac{\Delta t}{4})\frac{\Delta t}{2}$, (115b)<br>$\theta_n(t+\frac{\Delta t}{2}) = \theta_n(t+\frac{\Delta t}{4}) + \dot{\theta}_n(t+\frac{\Delta t}{2})\frac{\Delta t}{4}$, (115c)<br><br>where $\dot{\theta}_n$ is expressed in Eq. 105c and $\dot{\varphi}_n$ is expressed in Eq. 105d. In theory it is possible to have a singular value<br><br>$\dot{R} = \frac{P}{m}$, (105a)<br>$\dot{P} = -\frac{\partial \mathcal{H}_0}{\partial R} - r_s \sum_{k=1}^{N^2-1} \frac{\partial \mathcal{H}_k}{\partial R}\Omega_k = -\frac{\partial H_s(R,P)}{\partial R}$, (105b)<br>$\dot{\theta}_n = \left(\frac{\partial H_s}{\partial \varphi_n}\frac{2}{\sin\theta_n} - \frac{\partial H_s}{\partial \varphi_{n-1}}\tan\frac{\theta_n}{2}\right) \Big/ \left(r_s \prod_{j=1}^{n-1}\sin^2\frac{\theta_j}{2}\right)$, (105c)<br>$\dot{\varphi}_n = \frac{\dot{\Omega}_{\beta_{n+1,n}}\Omega_{\alpha_{n+1,n}} - \Omega_{\beta_{n+1,n}}\dot{\Omega}_{\alpha_{n+1,n}}}{\Omega^2_{\alpha_{n+1,n}} + \Omega^2_{\beta_{n+1,n}}}$. (105d) | ditions and the procedure are described in Sec. IV C. To propagate the dynamics, we use the simple Verlet algorithm because of the conjugate relation between $\Theta_n$ and $\varphi_n$ (see Eq. E5), as well as the relation between $\dot{\Theta}_n$ and $\dot{\theta}_n$ in Eq. E5a (to use the EOMs in Eq. E9).<br><br>First, the generalized conjugate variables $\{\varphi_n, \Theta_n\}$ are propagated by a half time-step, which is done using the Verlet algorithm as follows<br><br>$\Theta_n(t+\frac{\Delta t}{4}) = \Theta_n(t) + \dot{\Theta}_n(t)\frac{\Delta t}{4}$, (106a)<br>$\varphi_n(t+\frac{\Delta t}{2}) = \varphi_n(t) + \dot{\varphi}_n(t+\frac{\Delta t}{4})\frac{\Delta t}{2}$, (106b)<br>$\Theta_n(t+\frac{\Delta t}{2}) = \Theta_n(t+\frac{\Delta t}{4}) + \dot{\Theta}_n(t+\frac{\Delta t}{2})\frac{\Delta t}{4}$, (106c)<br><br>or equivalently with $\theta_n$ instead of $\Theta_n$, where $\dot{\theta}_n$ and $\dot{\varphi}_n$ are expressed in Eq. E9a-E9b and $\dot{\Theta}_n$ and $\dot{\varphi}_n$ in Eq. C8a-C8b. In theory it is possible to have a singular value for<br><br>$\dot{\theta}_n = \left(\frac{\partial H_s}{\partial \varphi_n}\frac{2}{\sin\theta_n} - \frac{\partial H_s}{\partial \varphi_{n-1}}\tan\frac{\theta_n}{2}\right) \Big/ \left(r_s \prod_{j=1}^{n-1}\sin^2\frac{\theta_j}{2}\right)$, (E9a)<br>$\dot{\varphi}_n = \frac{\dot{\Omega}_{\beta_{n+1,n}}\Omega_{\alpha_{n+1,n}} - \Omega_{\beta_{n+1,n}}\dot{\Omega}_{\alpha_{n+1,n}}}{\Omega^2_{\alpha_{n+1,n}} + \Omega^2_{\beta_{n+1,n}}}$, (E9b) |

The methods used to generate the figures, as Huo and his coworkers stated:

**Table 5: Details of Version 1 and Version 2**

| **From Version 1 (first released online to ChemRxiv on May 20, 2022)** | **From Version 2 (first released online to ChemRxiv on July 29, 2022)** |
|---|---|
| **VII. RESULTS AND DISCUSSIONS**<br><br>In this section, we refer to the linearized method in the $\mathfrak{su}(N)$ mapping formalism as the spin mapping (SM) approach, with the EOMs described in Eq. 94, or equivalently, in Eq. 105 or in Eq. 109. Here, we compare the<br><br>$\dot{R} = \frac{P}{m}$, (94a)<br>$\dot{P} = -\frac{\partial \mathcal{H}_0}{\partial R} - r_s \sum_{k=1}^{N^2-1} \frac{\partial \mathcal{H}_k}{\partial R}\Omega_k = -\frac{\partial H_s(R,P)}{\partial R}$, (94b)<br>$\frac{\mathrm{d}}{\mathrm{d}t}\Omega_i = \frac{1}{\hbar}\sum_{j,k=1}^{N^2-1} f_{ijk}\mathcal{H}_j\Omega_k$, (94c) | **VIII. RESULTS AND DISCUSSIONS**<br><br>In this section, we refer to the linearized method in the $SU(N)$ mapping formalism as the spin mapping (SM) approach, with the EOMs described in Eq. 98, or equivalently, in Eq. 113 or in Eq. 117. Here, we compare the<br><br>$\dot{R} = \frac{P}{m}$, (98a)<br>$\dot{P} = -\frac{\partial \mathcal{H}_0}{\partial R} - r_s \sum_{k=1}^{N^2-1} \frac{\partial \mathcal{H}_k}{\partial R}\Omega_k = -\frac{\partial H_s(R,P)}{\partial R}$, (98b)<br>$\frac{\mathrm{d}}{\mathrm{d}t}\Omega_i = \frac{1}{\hbar}\sum_{j,k=1}^{N^2-1} f_{ijk}\mathcal{H}_j(R)\Omega_k$, (98c) |

<table>
<tr><td>

$$\dot{R} = \frac{P}{m}, \tag{105a}$$

$$\dot{P} = -\frac{\partial \mathcal{H}_0}{\partial R} - r_s \sum_{k=1}^{N^2-1} \frac{\partial \mathcal{H}_k}{\partial R}\Omega_k = -\frac{\partial H_s(R,P)}{\partial R}, \tag{105b}$$

$$\dot{\theta}_n = \left(\frac{\partial H_s}{\partial \varphi_n}\frac{2}{\sin\theta_n} - \frac{\partial H_s}{\partial \varphi_{n-1}}\tan\frac{\theta_n}{2}\right) \Big/ \left(r_s \prod_{j=1}^{n-1}\sin^2\frac{\theta_j}{2}\right), \tag{105c}$$

$$\dot{\varphi}_n = \frac{\dot{\Omega}_{\beta_{n+1,n}}\Omega_{\alpha_{n+1,n}} - \Omega_{\beta_{n+1,n}}\dot{\Omega}_{\alpha_{n+1,n}}}{\Omega^2_{\alpha_{n+1,n}} + \Omega^2_{\beta_{n+1,n}}}. \tag{105d}$$

$$\dot{q}_n = \sum_m V_{nm}(R)\cdot p_m = \frac{\partial \mathcal{H}}{\partial p_n}, \tag{109a}$$

$$\dot{p}_n = -\sum_m V_{nm}(R)\cdot q_m = -\frac{\partial \mathcal{H}}{\partial q_m}. \tag{109b}$$

</td><td>

$$\dot{\theta}_n = \left(\frac{\partial H_s}{\partial \varphi_n}\frac{2}{\sin\theta_n} - \frac{\partial H_s}{\partial \varphi_{n-1}}\tan\frac{\theta_n}{2}\right) \Big/ \left(r_s \prod_{j=1}^{n-1}\sin^2\frac{\theta_j}{2}\right), \tag{113a}$$

$$\dot{\varphi}_n = \frac{\dot{\Omega}_{\beta_{n+1,n}}\Omega_{\alpha_{n+1,n}} - \Omega_{\beta_{n+1,n}}\dot{\Omega}_{\alpha_{n+1,n}}}{\Omega^2_{\alpha_{n+1,n}} + \Omega^2_{\beta_{n+1,n}}}, \tag{113b}$$

$$\dot{q}_n = \sum_m V_{nm}(R)\cdot p_m = \frac{\partial \mathcal{H}}{\partial p_n}, \tag{117a}$$

$$\dot{p}_n = -\sum_m V_{nm}(R)\cdot q_m = -\frac{\partial \mathcal{H}}{\partial q_m}. \tag{117b}$$

</td></tr>
</table>

**Table 6: Details of Version 1 and Version 3**

<table>
<tr><th>Version 1 (first released online to ChemRxiv on May 20, 2022)</th><th>Version 3 (accepted online on July 29, 2022)</th></tr>
<tr><td>

**VII. RESULTS AND DISCUSSIONS**

In this section, we refer to the linearized method in the $\mathfrak{su}(N)$ mapping formalism as the spin mapping (SM) approach, with the EOMs described in Eq. 94, or equivalently, in Eq. 105 or in Eq. 109. Here, we compare the

$$\dot{R} = \frac{P}{m}, \tag{94a}$$

$$\dot{P} = -\frac{\partial \mathcal{H}_0}{\partial R} - r_s \sum_{k=1}^{N^2-1} \frac{\partial \mathcal{H}_k}{\partial R}\Omega_k = -\frac{\partial H_s(R,P)}{\partial R}, \tag{94b}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\Omega_i = \frac{1}{\hbar}\sum_{j,k=1}^{N^2-1} f_{ijk}\mathcal{H}_j\Omega_k, \tag{94c}$$

</td><td>

**VIII. RESULTS AND DISCUSSIONS**

In this section, we refer to the linearized method in the $SU(N)$ mapping formalism as the spin mapping (SM) approach, with the EOMs described in Eq. 86, or equivalently, in Eq. E9 or in Eq. 95. Here, we compare the nu-

$$\dot{R} = \frac{P}{m}, \tag{86a}$$

$$\dot{P} = -\frac{\partial \mathcal{H}_0}{\partial R} - r_s \sum_{k=1}^{N^2-1} \frac{\partial \mathcal{H}_k}{\partial R}\Omega_k = -\frac{\partial H_s(R,P)}{\partial R}, \tag{86b}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\Omega_i = \frac{1}{\hbar}\sum_{j,k=1}^{N^2-1} f_{ijk}\mathcal{H}_j(R)\Omega_k, \tag{86c}$$

$$\dot{\theta}_n = \left(\frac{\partial H_s}{\partial \varphi_n}\frac{2}{\sin\theta_n} - \frac{\partial H_s}{\partial \varphi_{n-1}}\tan\frac{\theta_n}{2}\right) \Big/ \left(r_s \prod_{j=1}^{n-1}\sin^2\frac{\theta_j}{2}\right), \tag{E9a}$$

$$\dot{\varphi}_n = \frac{\dot{\Omega}_{\beta_{n+1,n}}\Omega_{\alpha_{n+1,n}} - \Omega_{\beta_{n+1,n}}\dot{\Omega}_{\alpha_{n+1,n}}}{\Omega^2_{\alpha_{n+1,n}} + \Omega^2_{\beta_{n+1,n}}}, \tag{E9b}$$

</td></tr>
</table>

| | |
|---|---|
| $$\dot{R} = \frac{P}{m}, \tag{105a}$$ $$\dot{P} = -\frac{\partial \mathcal{H}_0}{\partial R} - r_{\mathrm{s}} \sum_{k=1}^{N^2-1} \frac{\partial \mathcal{H}_k}{\partial R} \Omega_k = -\frac{\partial H_{\mathrm{s}}(R,P)}{\partial R}, \tag{105b}$$ $$\dot{\theta}_n = \Big(\frac{\partial H_{\mathrm{s}}}{\partial \varphi_n} \frac{2}{\sin\theta_n} - \frac{\partial H_{\mathrm{s}}}{\partial \varphi_{n-1}} \tan\frac{\theta_n}{2}\Big) \Big/ \Big(r_{\mathrm{s}} \prod_{j=1}^{n-1} \sin^2\frac{\theta_j}{2}\Big), \tag{105c}$$ $$\dot{\varphi}_n = \frac{\dot{\Omega}_{\beta_{n+1,n}} \Omega_{\alpha_{n+1,n}} - \Omega_{\beta_{n+1,n}} \dot{\Omega}_{\alpha_{n+1,n}}}{\Omega^2_{\alpha_{n+1,n}} + \Omega^2_{\beta_{n+1,n}}}. \tag{105d}$$ $$\dot{q}_n = \sum_m V_{nm}(R) \cdot p_m = \frac{\partial \mathcal{H}}{\partial p_n}, \tag{109a}$$ $$\dot{p}_n = -\sum_m V_{nm}(R) \cdot q_m = -\frac{\partial \mathcal{H}}{\partial q_m}. \tag{109b}$$ | $$\dot{q}_n = \sum_m V_{nm}(R) \cdot p_m = \frac{\partial \mathcal{H}}{\partial p_n}, \tag{95a}$$ $$\dot{p}_n = -\sum_m V_{nm}(R) \cdot q_m = -\frac{\partial \mathcal{H}}{\partial q_m}. \tag{95b}$$ |