

# Typo Corrections:

## Quantum Dynamics in Multistate Harmonic Models using Tensor-Train Thermofield Dynamics and Semiclassical Mapping Dynamics

Hao Zeng and Xiang Sun<sup>a)</sup>

*J. Chem. Phys.* **163**, 024131 (2025) DOI: [10.1063/5.0276946](https://doi.org/10.1063/5.0276946)

### I. TYPO CORRECTIONS

#### 1. Position: Page 9, Table I

##### Published version:

TABLE I. Model parameters of MSH models S1–S9(c) and N1–N8, with energy unit in  $\text{cm}^{-1}$ . MSH models S1–S9(a, b, d, e) sets are tuned from (c) set:  $\omega_c$ ,  $\Gamma_a$  and  $\Gamma_b$  are half for (a) set;  $\omega_c$ ,  $\Gamma_a$  and  $\Gamma_b$  are three times for (e) set;  $s^2$  and  $\varepsilon$  are three times for (b) set;  $s^2$  and  $\varepsilon$  are half for (d) set.

| Model | Equivalent      | $\omega_c$ | $s^2$ | $\varepsilon$ | $\Gamma_a$ | $\Gamma_b$ | $T / \text{K}$ |
|-------|-----------------|------------|-------|---------------|------------|------------|----------------|
| ...   |                 |            |       |               |            |            |                |
| N1    | #1 <sup>1</sup> | 10         | 0.5   | 100           | 100        | 10         | 0, 77, 300     |
| N2    | S2(d)           | 10         | 5     | 10            | 8          | 3          | 0, 4, 77, 300  |
| N3    | S5(d)           | 10         | 5     | 10            | 20         | 6          | 0, 77, 300     |
| N4    | S7(c)           | 30         | 50    | 20            | 120        | 45         | 0, 77, 300     |
| N5    | #2 <sup>1</sup> | 10         | 4.5   | 100           | 100        | 10         | 0, 77, 300     |
| N6    | #3 <sup>1</sup> | 10         | 50    | 100           | 100        | 10         | 0, 77, 300     |
| N7    | S9(a)           | 5          | 5     | 20            | 20         | 7.5        | 0, 77, 300     |
| N8    | S3(c)           | 30         | 5     | 20            | 24         | 9          | 0, 77, 300     |

##### Corrected:

TABLE II. Model parameters of MSH models S1–S9(c) and N1–N8, with energy unit in  $\text{cm}^{-1}$ . MSH models S1–S9(a, b, d, e) sets are tuned from (c) set:  $\omega_c$ ,  $\Gamma_a$  and  $\Gamma_b$  are half for (a) set;  $\omega_c$ ,  $\Gamma_a$  and  $\Gamma_b$  are three times for (e) set;  $s^2$  and  $\varepsilon$  are three times for (b) set;  $s^2$  and  $\varepsilon$  are half for (d) set.

| Model | Equivalent      | $\omega_c$ | $s^2$ | $\varepsilon$ | $\Gamma_a$ | $\Gamma_b$ | $T / \text{K}$ |
|-------|-----------------|------------|-------|---------------|------------|------------|----------------|
| ...   |                 |            |       |               |            |            |                |
| N1    | #1 <sup>1</sup> | 10         | 0.25  | 100           | 100        | 10         | 0, 77, 300     |
| N2    | S2(d)           | 10         | 5     | 10            | 8          | 3          | 0, 4, 77, 300  |
| N3    | S5(d)           | 10         | 5     | 10            | 20         | 6          | 0, 77, 300     |
| N4    | S7(c)           | 30         | 50    | 20            | 120        | 45         | 0, 77, 300     |
| N5    |                 | 10         | 2.25  | 100           | 100        | 10         | 0, 77, 300     |
| N6    |                 | 10         | 25    | 100           | 100        | 10         | 0, 77, 300     |
| N7    | S9(a)           | 5          | 5     | 20            | 20         | 7.5        | 0, 77, 300     |
| N8    | S3(c)           | 30         | 5     | 20            | 24         | 9          | 0, 77, 300     |

**Comment:** The model N5 and N6 are not #2 and #3 in Ref. 1, but labeled as MSH 2 and 3 in the internal test. The  $s^2$  for MSH N1, N5, and N6 are wrongly reported as twice the true value, which is already corrected in Ref. 2.

### REFERENCES

<sup>1</sup>H. Zeng, Y. Kou, and X. Sun, “How Sophisticated Are Neural Networks Needed to Predict Long-Term Nonadiabatic Dynamics?” *J. Chem. Theory Comput.* **20**, 9832–9848 (2024).

<sup>a)</sup>Electronic mail: [xiang.sun@nyu.edu](mailto:xiang.sun@nyu.edu)

<sup>2</sup>H. Zeng and X. Sun, “Estimating Memory Time within the Frameworks of Generalized Quantum Master Equation and Transfer Tensor Methods,” J. Chem. Phys. **164**, 224117 (2026).