

Typo Corrections:

Data-Driven Versus Physics-Informed Neural Networks for Nonadiabatic Semiclassical Mapping Dynamics

Hao Zeng and Xiang Sun^{a)}

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I. TYPO CORRECTIONS

1. Position: Page 219, Eq. (2)

Published version:

$$H(\mathbf{P}, \mathbf{R}, \mathbf{p}, \mathbf{q}) \quad (1)$$

$$= \frac{\mathbf{P}^2}{2\mu} + \sum_{j,k}^F V_{jk}(\mathbf{R}) \left[\frac{1}{2\hbar} (q_i - ip_j) \times (q_k + ip_k) - \gamma \delta_{jk} \right], \quad (2)$$

Corrected:

$$H(\mathbf{P}, \mathbf{R}, \mathbf{p}, \mathbf{q}) \quad (3)$$

$$= \frac{\mathbf{P}^2}{2\mu} + \sum_{j,k}^F V_{jk}(\mathbf{R}) \left[\frac{1}{2\hbar} (q_j - ip_j) \times (q_k + ip_k) - \gamma \delta_{jk} \right], \quad (4)$$

Comment: It was correct in our LaTeX document; however, it was wrong in the proof and was not found at that time.

2. Position: Page 220, Eqs. (16)–(18)

Published version:

In the CMM method [18-22], the mapping variables $(\mathbf{q}, \mathbf{p})$ are sampled on a $(2F-1)$ -sphere to satisfy the condition that the total electronic population equals one:

$$S(\gamma): \sum_{j=1}^F \frac{1}{2\hbar} (q_j^2 + p_j^2) = 1 + F\gamma. \quad (16)$$

The electronic observables at time 0 and t are given by

$$M_{jk}^{(0)}(\mathbf{q}, \mathbf{p}) = \frac{1}{2\hbar} (q_j - ip_j)(q_k + ip_k) - \gamma \delta_{jk}, \quad (17)$$

$$M_{jk}^{(t)}(\mathbf{q}, \mathbf{p}) = \frac{\mathcal{Q}_{jk}(\bar{\gamma}, \gamma)}{2\hbar} (q_j - ip_j)(q_k + ip_k) - \bar{\gamma} \delta_{jk}, \quad (18)$$

Corrected:

$$S(\gamma): \sum_{j=1}^F \frac{1}{2\hbar} (q_j^2 + p_j^2) = 1 + F\gamma. \quad (5)$$

$$M_{jk}^{(0)}(\mathbf{q}, \mathbf{p}) = \frac{1}{2\hbar} (q_j - ip_j)(q_k + ip_k) - \gamma \delta_{jk}, \quad (6)$$

^{a)}Electronic mail: xiang.sun@nyu.edu

$$M_{jk}^{(t)}(\mathbf{q}, \mathbf{p}) = \frac{Q(\bar{\gamma}, \gamma)}{2\hbar} (q_j - ip_j)(q_k + ip_k) - \bar{\gamma} \delta_{jk}, \quad (7)$$

Comment: The “ $\hbar$ ” were correct in our manuscript, but are wrongly rendered in the published version.