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Erratum: "Non-adiabatic mapping dynamics in the phase space of the $SU(N)$ Lie group" [J. Chem. Phys. 157, 084105 (2022)]

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I. CORRECTION IN THE SURFACE HOPPING RESULTS IN FIG. 4

After publishing the paper (Ref. 1), unfortunately, we noticed an error that was generated when we digitize the fewest switches surface hopping (FSSH) result from Ref. 2. This digitization error leads to an incorrect FSSH result in Fig. 4(c) of the original paper (Ref. 1). Here, we provide the correct version of this figure. The only change made in this figure is the FSSH result, shown in the dashed lines in panel (c) of Fig. 1. Compared to the original version of Fig. 4 in Ref. 1, the state 3 population [the green dashed curve in panel (c)] obtained from FSSH is closer to the exact results [the green solid curve in panel (c)]. Our main conclusion drawn in the original paper (Ref. 1), which is that the spin mapping (SM) approach [panels (b) and (d)] outperforms the FSSH method [in panel (c)] for this particular model system, remains unaffected, as the FSSH result (in Ref. 2) provides significantly less accurate population dynamics for states 1 [the red dashed line in panel (c)] and 2 [the blue dashed line in panel (c)].

II. CLARIFICATION ON THE NUMERICAL ALGORITHM USED TO PROPAGATE DYNAMICS

We want to clarify the numerical algorithm we used to propagate the EOMs and generate all numerical results presented in the paper. As opposed to Eq. (106) in the main text, the numerical algorithm we used to generate all numerical results is actually based on the following integration[3] of $\{\theta_n, \varphi_n\}$:

$$\boldsymbol{\theta}\left(t+\frac{\Delta t}{4}\right)=\boldsymbol{\theta}(t)+\dot{\boldsymbol{\theta}}(t)\frac{\Delta t}{4}, \tag{1a}$$

$$\boldsymbol{\varphi}\left(t+\frac{\Delta t}{2}\right)=\boldsymbol{\varphi}(t)+\dot{\boldsymbol{\varphi}}\left(t+\frac{\Delta t}{4}\right)\frac{\Delta t}{2}, \tag{1b}$$

$$\boldsymbol{\theta}\left(t+\frac{\Delta t}{2}\right)=\boldsymbol{\theta}\left(t+\frac{\Delta t}{4}\right)+\dot{\boldsymbol{\theta}}\left(t+\frac{\Delta t}{2}\right)\frac{\Delta t}{4}. \tag{1c}$$

To integrate the above equations, we need the expressions of the time-derivatives of θ_n and φ_n [Eq. (E9)],

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

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

where, for $n = 1$, the denominator is replaced by r_s because there is no θ_0 variable and the numerator only has the term that includes $\frac{\partial H_s}{\partial\varphi_n}$ as there is no φ_{n-1}. In the above expressions, to compute $\frac{\partial H_s}{\partial\varphi_n}$, we use Eq. (C2) of the paper. To compute $\dot{\Omega}_{\alpha_{k,n}}$ and $\dot{\Omega}_{\beta_{kn}}$, we use Eqs. (C5) and (C6) of the paper, respectively. To evaluate terms related to $\{\Omega_n\}$, we use Eqs. (B2)–(B4) of the paper.

To compute the population dynamics, we use the estimator expressed in terms of $\{\theta_n\}$, which is Eq. (62) of the paper,

$$[|n\rangle\langle n|]_s=\frac{1}{N}+r_s\left(-\frac{1}{N}+\cos^2\frac{\theta_n}{2}\prod_{k=1}^{n-1}\sin^2\frac{\theta_k}{2}\right). \tag{3}$$

As we have already emphasized in the paper, an *alternative* but *numerically simpler* way to propagate dynamics is to directly

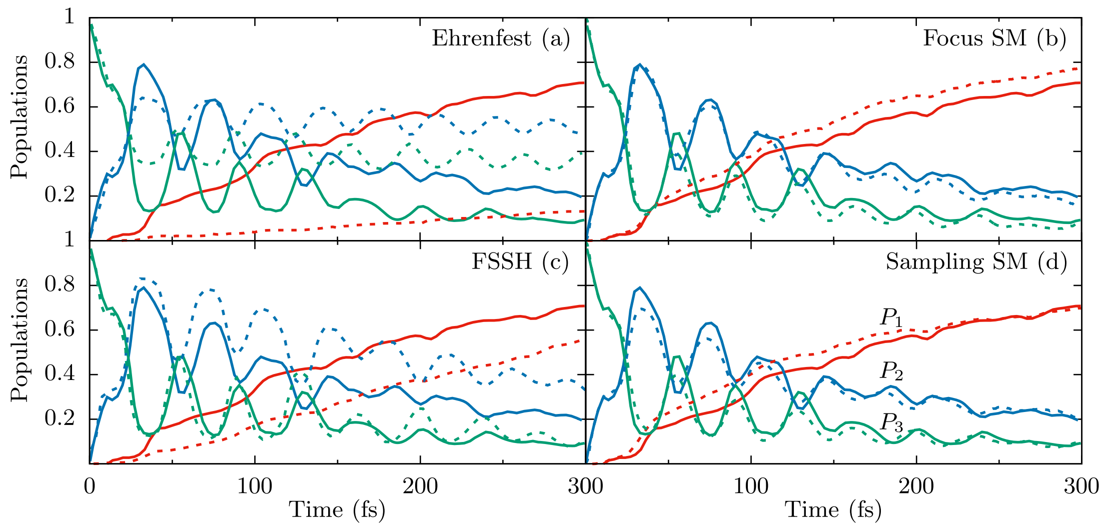

FIG. 1. Corrected version of Fig. 4 in the paper. A correction is made only to the result of the FSSH population dynamics in panel (c), which is now correctly digitized from Ref. 2.

propagate the EOMs with the MMST variables [see Eq. (95) of the paper]. This is an *easier approach to implement into computer code*, because these equations [Eq. (95) of the paper] are simpler than the corresponding EOMs for $\{\varphi_n, \theta_n\}$. In addition, there are several previously developed symplectic integrators[4,5] to propagate these EOMs, which one can take advantage of. Our numerical tests confirm that identical results are obtained using this approach. This is an independent test of the validity of the algorithm in Eqs. (1)–(3) of this erratum.

III. CLARIFICATION ON THE NOTE IN REF. 65

In the published paper (Ref. 1), we have put a note (Ref. 65 in the original paper[1]) stating that "To the best of our knowledge, we do not see this expression in the previous literature." This expression refers to Eq. (27) of the main text in Ref. 1, expressed as follows:

$$\hat{w}_s(\boldsymbol{\Omega}) = \frac{1 - r_s}{N}\hat{\mathcal{I}} + r_s|\boldsymbol{\Omega}\rangle\langle\boldsymbol{\Omega}|. \tag{4}$$

We did not realize until recently that this simple equation was discovered in Ref. 6, which is Eq. (4.7) and is expressed as

$$\begin{aligned} F^{s'}_{N,1}(\boldsymbol{\theta},\boldsymbol{\varphi}) &= \frac{\Omega(s')}{\Omega(s)}\widetilde{F}^{s}_{N,1}(\boldsymbol{\theta},\boldsymbol{\varphi}) + \frac{1}{N}\mathbb{I}_N \\ &= \frac{\Omega(s')}{\Omega(s)}\left(F^{s}_{N,1}(\boldsymbol{\theta},\boldsymbol{\varphi}) - \frac{1}{N}\mathbb{I}_N\right) + \frac{1}{N}\mathbb{I}_N \\ &= \frac{\Omega(s')}{\Omega(s)}F^{s}_{N,1}(\boldsymbol{\theta},\boldsymbol{\varphi}) + \left(1 - \frac{\Omega(s')}{\Omega(s)}\right)\frac{1}{N}\mathbb{I}_N, \end{aligned} \tag{5}$$

where $F^{s}_{N,1}(\boldsymbol{\theta},\boldsymbol{\varphi})$ is the generating kernel of Stratonovich–Weyl correspondence that depends on the value of s. Furthermore, $\Omega(s)$ in Eq. (5) [cf. Eq. (3.16) of Ref. 6] is expressed as follows:

$$\Omega(s) = \begin{cases} \sqrt{N+1}, & s = 0, \\ 1, & s = +1, \\ N+1, & s = -1. \end{cases} \tag{6}$$

The above $\Omega(s)$ expression, which defines finite-dimensional Wigner, Q-, and P-functions of the $SU(N)$-symmetric quasi-probability distribution, plays the same role as our Bloch sphere radius r_s in our work Ref. 1.

If one takes the following substitutions:

$$r_{s'} \equiv \frac{\Omega(s')}{\Omega(s)}, \quad |\boldsymbol{\Omega}\rangle\langle\boldsymbol{\Omega}| \equiv F^{s}_{N,1}(\boldsymbol{\theta},\boldsymbol{\varphi}), \quad \text{and} \quad s = +1, \tag{7}$$

then Eq. (5) is identical to Eq. (4). We apologize for our limited knowledge at the time when we wrote this particular note. We want to clarify that Ref. 6 was the first work that discovered this expression.

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