

**Typos in MInt paper (Nonadiabatic semiclassical dynamics in the mixed quantum-classical initial value representation; M. S. Church, T. J. H. Hele, G. S. Ezra and N. Ananth; J. Chem. Phys., 148 (2018), 102326)**

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1. Appendix B, Section 3: Step 8 of the algorithm should be  
\*From Eq. (B14), find  $M_{px}$  and  $M_{pp}$  using  $\{E_k\}$  and  $\{F_k\}$  from step 5.
2. Appendix E, Section 3. The Split Liouvillian (SL) Algorithm: E17 should be

$$\begin{bmatrix} 1 & \mathbf{0}^T & 0 & \mathbf{0}^T \\ \mathbf{0} & \mathbb{I} & \mathbf{0} & \mathbb{O} \\ \tilde{\mathbf{b}} & -\mathbf{x}^T \mathbf{V}' \Delta t & 1 & -\mathbf{p}^T \mathbf{V}' \Delta t \\ \mathbf{0} & \mathbb{O} & \mathbf{0} & \mathbb{I} \end{bmatrix}$$

3. Appendix E, Section 3. The SL Algorithm: E19 should be

$$\tilde{\mathbf{b}} := -\frac{1}{2}(\mathbf{x}^T \mathbf{V}'' \mathbf{x} + \mathbf{p}^T \mathbf{V}'' \mathbf{p} - \text{Tr}[\mathbf{V}'']) \Delta t$$

4. Appendix E, Section 3. The SL Algorithm: E21 should be

$$\begin{bmatrix} 0 & -\mathbf{g}^T \mathbf{D} + \mathbf{f}^T \mathbf{C} & -1 & -\mathbf{g}^T \mathbf{C} - \mathbf{f}^T \mathbf{D} \\ -\mathbf{Cf} + \mathbf{Dg} & \mathbb{O} & \mathbf{0} & -\mathbb{I} \\ \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{Df} + \mathbf{Cg} & \mathbb{I} & \mathbf{0} & \mathbb{O} \end{bmatrix} = \begin{bmatrix} 0 & e & -1 & a \\ -e^T & \mathbb{O} & \mathbf{0} & -\mathbb{I} \\ \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ -a^T & \mathbb{I} & \mathbf{0} & \mathbb{O} \end{bmatrix}$$

5. Appendix E, Section 3. The SL Algorithm: E22 should be

$$\begin{bmatrix} 1 & \mathbf{0}^T & 0 & \mathbf{0}^T \\ g & \mathbf{C} & \mathbf{0} & -\mathbf{D} \\ \tilde{\mathbf{b}} & -\mathbf{x}^T \mathbf{V}' \Delta t & 1 & -\mathbf{p}^T \mathbf{V}' \Delta t \\ f & \mathbf{D} & \mathbf{0} & \mathbf{C} \end{bmatrix}$$

6. Appendix E, Section 3. The SL Algorithm: E24 should be

$$\begin{bmatrix} 1 & \mathbf{0}^T & 0 & \mathbf{0}^T \\ g & \mathbf{C} & \mathbf{0} & -\mathbf{D} \\ \tilde{\mathbf{b}} & \tilde{e} & 1 & \tilde{a} \\ f & \mathbf{D} & \mathbf{0} & \mathbf{C} \end{bmatrix}$$

None of these typos in any way affect the validity of the scientific results in the paper, namely that the MInt algorithm is symplectic whereas the SL algorithm is not.