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Erratum: "How to recover Marcus theory with fewest switches surface hopping: Add just a touch of decoherence" [J. Chem. Phys.137, 22A513 (2012)]

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Erratum: "How to recover Marcus theory with fewest switches surface hopping: Add just a touch of decoherence" [J. Chem. Phys. 137, 22A513 (2012)]

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Equation (45) of the paper[1] should read

$$c_j^{\text{new}} = \begin{cases} c_j & j \neq n, j \neq i \\ \frac{c_i}{|c_i|}\sqrt{|c_i|^2 + |c_n|^2} & j = i \\ 0 & j = n \end{cases}$$

This collapsing and renormalization scheme is necessary to maintain consistency between the electronic amplitudes and the number of trajectories on each surface. For the case of multiple electronic states (as in Ref. 37), our algorithm was successfully benchmarked using this corrected scheme.

[1]B. R. Landry and J. E. Subotnik, J. Chem. Phys. **137**, 22A513 (2012).

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