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# A simple way to deal with decoherence in trajectory surface hopping

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Tully's fewest switches surface hopping is a leading computational method for excited-state dynamics in molecules and materials. It unfortunately lacks a proper description of decoherence, which has lead to numerous "decoherence correction" schemes. However, the by far most commonly used "energy-based correction" is not guaranteed to improve accuracy - in fact, it often even harms more than it helps. The problem is that it relies on a parameter that assumes a given energy scale, and therefore only works for systems that are similar to those the method was originally tested on.
As a simple way to avoid this problem, I suggest to restrict decoherence to regions of low nonadiabaticity measured by the Massey parameter [1]. The advantage of this criterion is that the threshold is dimensionless, so the same value is suitable for a variety of systems with vastly different size and absolute energy scales, which I will demonstrate with a suite of benchmark systems including conical intersection system, condensed-phase models, photosynthetic complexes, and molecules with spin-orbit coupling. I will also show how the method helps describe charge conduction in periodic molecular crystals [2]. The method adds minimal computational effort and the results are relevant for any surface-hopping simulations of excited-state dynamics in complex systems.

[1] J.E. Runeson, J. Chem. Phys. 163, 154105 (2025).
[2] J.E. Runeson, T.J.G. Drayton, and D.E. Manolopoulos, J. Chem. Phys. 161, 144102 (2024).