Canonically consistent quantum master equation for proton-transfer reactions

Zahra Sartipi,[1,*] Richard Gundermann,[2]
Janet Anders,[1,3] and Peter Saalfrank[2]

[1] *Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany*
[2] *Institute of Chemistry, University of Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany*
[3] *Department of Physics and Astronomy, University of Exeter, Exeter EX4 4QL, United Kingdom*

We investigate intramolecular proton transfer in thioacetylacetone (TAA, C_4H_6OS) using the canonically consistent quantum master equation (CCQME). The molecule is modeled as an N-level quantum system coupled to a solvent environment represented by a harmonic bath with an Ohmic–Drude spectral density. The performance of the CCQME is examined in comparison with the Redfield master equation. We also implemented the numerically exact hierarchical equations of motion (HEOM) calculations as the benchmark reference. The results show that the Redfield description deviates from the HEOM results as the system–bath coupling strength increases, whereas the CCQME remains in good agreement with the exact HEOM benchmark up to the intermediate-coupling regime.

* zahra.sartipi@uni-potsdam.de