

Abstract Submitted
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Modeling Quantum Dynamics in Multidimensional Systems

KYLE LISS, Dickinson College, THOMAS WEINACHT, Stony Brook University, BRETT PEARSON, Dickinson College — Coupling between different degrees-of-freedom is an inherent aspect of dynamics in multidimensional quantum systems. As experiments and theory begin to tackle larger molecular structures and environments, models that account for vibrational and/or electronic couplings are essential for interpretation. Relevant processes include intramolecular vibrational relaxation, conical intersections, and system-bath coupling. We describe a set of simulations designed to model coupling processes in multidimensional molecular systems, focusing on models that provide insight and allow visualization of the dynamics. Undergraduates carried out much of the work as part of a senior research project. In addition to the pedagogical value, the simulations allow for comparison between both explicit and implicit treatments of a system's many degrees-of-freedom.

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