

Abstract Submitted
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Quantum dynamics of molecular energy transfer using coupled operator algebras TIM WENDLER, GUS HART, MANUEL BERRONDO, Brigham Young University — The Schrodinger equation for the time-evolution operator is sufficient for calculating quantum dynamics of the perturbed harmonic vibrational states of a single chemical bond. It is shown to be easily extended to more complex molecular energy transfers such as molecular collisions and chemical reactions through the coupling of algebras. This application of Lie algebra, called the vibron model, is shown to produce results in the following 3 examples: 1) Carbon dioxide absorbing energy from an external electromagnetic field, 2) Collinear inelastic collision of a diatomic molecule with an incoming atom, and 3) Collinear reactive collision of the deuterium with methane.

Tim Wendler
Brigham Young University

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