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Quantum Control of Diatomic Molecular Vibration States Using Space-Time Discretization[1] CHARLES WEATHERFORD, XINGJUN ZHANG, Physics Department, Florida A&M University — Molecular evolution in an external field can be efficiently calculated by using our Space-Time algorithm (STA), which deploys a basis set in space and time and turns Quantum Mechanical initial-value problems into a set of simultaneous algebraic equations and can be used to simulate the control of the Quantum states of a molecule. The external field must be optimized so as to restrict the search space to those parameter values characterizing the field, which are available in experiments. A generalized evolution strategy is employed which provides a technique for parameter optimizations. We have developed a parallel algorithm which implements an evolution strategy using the STA to optimize the external field intensity (laser amplitude) so as to drive the molecule from an initial vibrational state to a desired vibrational state. We optimize the molecular evolution procedure in two ways: a step-by-step optimization and a closed-loop optimization. The method is applied to NO^+. The simulation has been done using 5 vibrational states.

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