

## **MCTDH Computations and the Quantum Markovian Master Equation for Scattering from Surfaces\***

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The Multi-configurational time dependent Hartree (MCTDH) method was employed to address the numerically exact 1-D scattering of Ar from a LiF surface at T=0 K. The Hamiltonian consisted of a Morse potential coupled to a bath of harmonic modes. The results were converged as a function of number of modes and compared to those obtained by an approximate Master equation. The comparison is quantitative - confirms the reliability of the Master equation in describing the scattering process. The Master equation provides insight into the quantum scattering process as a function of temperature and other variables. This is a first step towards developing a Master equation approach for the scattering of atoms from surfaces in 3-D.

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