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A Direct, Time Dependent, Lanczos Propagation Method for Non-Orthogonal Basis Sets BARRY I. SCHNEIDER, Physics Division, NSF, Arlington, VA 22230 and Electron and Optical Physics Division, NIST, Gaithersburg, MD 20899, XIAOXU GUAN, Drake University, Des Moines, IA 50311, JOHANNES FEIST, Institute for Theoretical Physics, Vienna Unversity of Technology, A1040, Vienna, Austria, KLAUS BARTSCHAT, Drake University, Des Moines, IA 50311, CLIFF NOBLE, CSED, Daresbury Laboratory, WA4 4AD, UK, OLEG ZATSARINNY, Drake University, Des Moines, IA 50311 — We have developed an efficient approach for solving the time-dependent Schroedinger equation for the interaction of a strong laser pulse with a general atom, when the many-electron basis set is non-orthogonal. The propagation equations have the form, iS dC(t) / dt = HC(t) where S and H are respectively the overlap and Hamiltonian matrices in the many-electron space. By a succession of Lanczos orthogonalizations, the Hamiltonian is reduced to tri-diagonal form, but the overlap matrix remains full in the small, Lanczos basis. Thus, we are faced with solving a small, generalized eigenvalue problem at each step of the Lanczos recursion. The approach is still dominated by the need to find an efficient way to multiply the H and S matrix on a vector. Some examples of the new method will be presented in the talk.

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