Title:	Quantum Dynamics with Explicitly Time-Dependent Hamiltonians in Multiple Time Scales: A New Algorithm for (t, t′) and (t, t′, t″) Methods in Laser–Matter Interactions
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Keywords:	Explicitly Time-Dependent Hamiltonians Quantum Dynamics
Issue Date:	2019
Publisher:	American Chemical Society
Citation:	Journal of Chemical Theory and Computation, 16(1).
Abstract:	The (t, t′) method for quantum dynamics with general time-dependent Hamiltonians is exact yet expensive to implement, in the context of laser–atom, laser–molecule interactions. The evolution operator requires a huge storage space with a large operation count for the propagation. A new method is suggested in this work where an analytical block diagonalization of the Floquet Hamiltonian is proposed. The block diagonalization in this novel algorithm is based on Chebyshev polynomials of the second kind. This is combined with a split operator method of chosen order to approximate the full evolution operator. The number of operations are drastically reduced to that of a matrix-vector multiplication repeated only to the order of the number of Floquet channels. Hence, only matrices of the order of the number of position basis functions need to be stored. Thus, the presented algorithm is an effective tool for solving the (t, t′, t″) problem for interactions with a bichromatic laser and a single-frequency laser pulse with explicit interactions of the pulse envelope. Hydrogen atom, helium, water, and ammonia, represented with Hamiltonians obtained from standard electronic structure packages, have been investigated in the presence of linearly polarized pulsed laser fields and bichromatic laser fields presenting various time-dependent properties from the program.
URI:	https://pubs.acs.org/doi/10.1021/acs.jctc.9b00863 (https://pubs.acs.org/doi/10.1021/acs.jctc.9b00863) http://hdl.handle.net/123456789/2327 (http://hdl.handle.net/123456789/2327)
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