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Use of Space-Time Basis Sets for Solving Initial-Value Problems[1]

CHARLES WEATHERFORD, XINGJUN ZHANG, Florida A&M University — A new algorithm for solving Quantum Mechanical initial-value problems such as the time-dependent Schroedinger equation and the Liouville equation is described. The method avoids the use of the time-translation operator which inevitably results in an essentially sequential algorithm and instead turns the problem into the solution of simultaneous equations, which produces a highly parallelizable algorithm. A basis set in time as well as spatial degrees of freedom is used. The basis may be spectral, finite element, or spectral element and may be continuous or discrete (discrete variable representation–DVR). The time-axis may have an arbitrary size of time element including only one element. The larger the time step, the larger the size of the time basis that is required. The Hamiltonian may be time-independent or time-dependent. In the case of a time-independent Hamiltonian, an extremely efficient algorithm results. For the time-dependent case, the problem of time-ordering does not arise. Several applications involving laser-atom interactions will be given.

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