Discretization of Time Dependent Quantum Systems: The Evolution Operators

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We discuss time dependent quantum systems. Our emphasis is on the linear problem, but our work may be viewed as a framework for several models, including linear iterations involved in time dependent density functional theory (TDDFT), the Hartree-Fock model, or other quantum models. A key aspect of the analysis of the algorithms is the use of time-ordered evolution operators, which allow for both a well-posed problem and its approximation. We discuss the available theory at the outset, and proceed to apply the theory systematically, via approximations. We discuss rigorous use of the rectangular and Gauss quadrature rules. Our work is consistent with first-principle, real-time propagation of electronic states, aimed at finding the non-linear responses of quantum systems. Given the increasing importance of quantum modeling in applications, we are attempting to identify some of the basic issues to be addressed analytically.