Highly accurate solution for inhomogeneous and homogeneous Schrödinger equations

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A great effort has been devoted in quantum dynamics to finding efficient and accurate numerical methods to solve the time-dependent Schrödinger equation. Inhomogeneous time-dependent Schrödinger equations arise for example in reactive scattering and in optimal control theory with time-dependent targets or state-dependent constraints.

First, we present a propagation scheme for time-dependent inhomogeneous Schrödinger equations [1]. A formal solution of the inhomogeneous Schrödinger equation is derived based on a polynomial expansion of the inhomogeneous term. This formal solution is adapted to a Chebychev propagation scheme. Different variants for the inhomogeneous propagator are demonstrated and applied to two examples from optimal control theory. Convergence behavior and numerical efficiency are analyzed.

Second, we introduce a novel algorithm to solve the homogeneous Schrödinger equation for explicitly time-dependent Hamiltonians based on iterative time-ordering. The basic idea consists in rewriting the time-dependence as an inhomogeneous term. In order to demonstrate the accuracy of the iterative time-ordering algorithm, analytically solvable examples are considered. The numerical efficiency is analyzed by comparison with the (t, t') [2] method.

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[1] M. Ndong, H. Tal-Ezer, R. Kosloff, and C. P. Koch, J. Chem. Phys. **130**, 124108-124119 (2009).

[2] U. Peskin, R. Kosloff, and N. Moiseyev, J. Chem. Phys. **100**, 8849-8855 (1994).