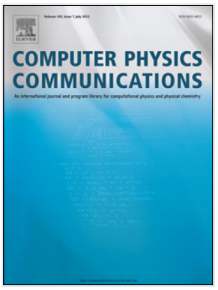
Accepted Manuscript



Single-step Propagators for calculation of time evolution in quantum systems with arbitrary interactions

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PII: S0010-4655(16)30021-2
DOI: http://dx.doi.org/10.1016/j.cpc.2016.02.006
Reference: COMPHY 5865

To appear in: *Computer Physics Communications*

Received date: 30 June 2015
Revised date: 31 December 2015
Accepted date: 9 February 2016

Please cite this article as: I. Gonoskov, M. Marklund, Single-step Propagators for calculation of time evolution in quantum systems with arbitrary interactions, *Computer Physics Communications* (2016), http://dx.doi.org/10.1016/j.cpc.2016.02.006

to Computer Physics Communications (revised)/

Single-step Propagators for calculation of time evolution in quantum systems with arbitrary interactions

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(Dated: December 31, 2015)

We propose and develop a general method of numerical calculation of the wave function time evolution in a quantum system which is described by Hamiltonian of an arbitrary dimensionality and with arbitrary interactions. For this, we obtain a general n-order single-step propagator in closed-form, which could be used for the numerical solving of the problem with any prescribed accuracy. We demonstrate the applicability of the proposed approach by considering a quantum problem with non-separable time-dependent Hamiltonian: the propagation of an electron in focused electromagnetic field with vortex electric field component.

I. INTRODUCTION

Theoretical analysis of quantum systems and their time evolution often leads to necessity of solving the corresponding partial differential equations with time-dependent Hamiltonians. For the typical problem, when the corresponding closed-form solution is unknown, a direct numerical calculation could be an efficient tool for obtaining the solution approximation with a reasonable (and sometimes controlled) accuracy level. The main aim of our manuscript is to develop a general way of the numerical implementation with controlled accuracy based on single-step finite-order propagators. Such numerical schemes represent a step-by-step repetition procedure for a number of steps corresponding to some certain time intervals. At each step, a new solution approximation is calculated, based on the previous one (or initial condition), and a certain operator: single-step propagator.

A derivation of the single-step propagators is usually based on a power series expansion of the corresponding solution approximation obtained from a perturbation theory or its analogues (see [1–4] and references therein). The particular propagators and the corresponding implementations further could be modified in a variety of ways, in order to increase the numerical efficiency for a certain problem. For example, for solving a time-dependent Schrödinger equation (TDSE) one of the most popular and well-known method is an *exponential split-operator technique* [1, 5], which correspond to a second-order solution approximation in the case of separable Hamiltonians. Other improvements could be achieved by using special expansions and specific references for the general solution approximation (for example, *harmonic-oscillator reference propagator* [3, 6]). However, the majority of these methods could not be straightforwardly adapted and efficiently implemented for the most general statement which includes arbitrary Hamiltonian structures and interaction potentials in the corresponding equations.

In this manuscript we propose and develop a numerical approach which is based on general single-step propagators. Such propagators allow to calculate a time evolution in the case of a most general statement: for arbitrary Hamiltonian structures and interaction potentials, and with any prescribed accuracy level. The derivation of the general propagator is based on the exact solution from cyclic operator decomposition (COD) [7]. This solution is used for the obtaining of the n-order solution approximation for a finite time interval in a closed-form. Final expression for the propagator represents the optimization of the corresponding approximation for the efficient numerical implementation.

The manuscript is organized as follows. After the introduction in Sec.I, we consider the exact solution, finite-order approximations and the corresponding propagators in Sec.II. In Sec.III we derive the general n-order single-step propagator. Next, in Sec.IV we consider several particular examples and corresponding optimizations for the *first-*, *second-*, and *third-order* propagators. After that, in Sec.V we compare accuracy of the numerical algorithms which are based on the derived propagators in case of numerical solving of TDSE with quadratic potential. In Sec.VI we apply the propagator's technique for the calculation in the case of non-separable Hamiltonian: namely, the interaction of the an electron in focused electromagnetic field with vortex electric field component. Sec.VII is devoted to conclusions.

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