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SPEEDUP Code for Calculation of Transition Amplitudes via the Effective Action Approach

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Abstract. We present Path Integral Monte Carlo C code for calculation of quantum mechanical transition amplitudes for 1D models. The SPEEDUP C code is based on the use of higher-order short-time effective actions and implemented to the maximal order p=18 in the time of propagation (Monte Carlo time step), which substantially improves the convergence of discretized amplitudes to their exact continuum values. Symbolic derivation of higher-order effective actions is implemented in SPEEDUP Mathematica codes, using the recursive Schrödinger equation approach. In addition to the general 1D quantum theory, developed Mathematica codes are capable of calculating effective actions for specific models, for general 2D and 3D potentials, as well as for a general many-body theory in arbitrary number of spatial dimensions.

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1 Introduction

Exact solution of a given many-body model in quantum mechanics is usually expressed in terms of eigenvalues and eigenfunction of its Hamiltonian

$$\hat{H}=\sum_{i=1}^{M}\frac{\hat{\mathbf{p}}_i^2}{2m_i}+\hat{V}(\hat{\mathbf{q}}_1,\cdots,\hat{\mathbf{q}}_M), \tag{1.1}$$

but it can be also expressed through analytic solution for general transition amplitude $A(\mathbf{a},\mathbf{b};T)=\langle\mathbf{b}|e^{-iT\hat{H}/\hbar}|\mathbf{a}\rangle$ from the initial state $|\mathbf{a}\rangle$ to the final state $|\mathbf{b}\rangle$ during the time of

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propagation T. Calculation of transition amplitudes is more suitable if one uses path integral formalism [1–3], but in principle, if eigenproblem of the Hamiltonian can be solved, one should be able to calculate general transition amplitudes, and vice versa. However, mathematical difficulties may prevent this, and even more importantly, exact solutions can be found only in a very limited number of cases. Therefore, use of various analytic approximation techniques or numerical treatment is necessary for detailed understanding of the behavior of almost all models of interest.

In numerical approaches it could be demanding and involved to translate numerical knowledge of transition amplitudes to (or from) eigenstates, but practically can be always achieved. It has been implemented in various setups, e.g. through extraction of the energy spectra from the partition function [2–5], and using the diagonalization of space-discretized matrix of the evolution operator, i.e. matrix of transition amplitudes [6–10]. All these applications use the imaginary-time formalism [11, 12], typical for numerical simulations of such systems.

Recently introduced effective action approach [13–17] provides an ideal framework for exact numerical calculation of quantum mechanical amplitudes. It gives systematic short-time expansion of amplitudes for a general potential, thus allowing accurate calculation of short-time properties of quantum systems directly, as has been demonstrated in [8–10]. For numerical calculations that require long times of propagation to be considered using e.g. Monte Carlo method, effective action approach provides improved discretized actions leading to the speedup in the convergence of numerically calculated discretized quantities to their exact continuum values. This has been also demonstrated in Monte Carlo calculations of energy expectation values using the improved energy estimators [5, 18].

In this paper we present SPEEDUP codes [19] which implement the effective action approach, and which were used for numerical simulations in [4, 5, 8–10, 13–17]. The paper is organized as follows. In Section 2 we briefly review the recursive approach for analytic derivation of higher-order effective actions. SPEEDUP Mathematica codes capable of symbolic derivation of effective actions for a general one- and many-body theory as well as for specific models is described in detail in Section 3, while in Section 4 we describe SPEEDUP Path Integral Monte Carlo C code, developed for numerical calculation of transition amplitudes for 1D models. Section 5 summarizes presented results and gives outlook for further development of the code.

2 Theoretical background

From inception of the path integral formalism, expansion of short-time amplitudes in the time of propagation was used for the definition of path integrals through the time-discretization procedure [2, 3]. This is also straightforwardly implemented in the Path Integral Monte Carlo approaches [20], where one usually relies on the naive discretization of the action. Several improved discretized actions, mainly based on the Trotter formula