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Numerical Path Integral Approach to Quantum Dynamics and Stationary Quantum States

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Abstract. Applicability of Feynman path integral approach to numerical simulations of quantum dynamics of an electron in real time domain is examined. Coherent quantum dynamics is demonstrated with one dimensional test cases (quantum dot models) and performance of the Trotter kernel as compared with the exact kernels is tested. Also, a novel approach for finding the ground state and other stationary sates is presented. This is based on the incoherent propagation in real time. For both approaches the Monte Carlo grid and sampling are tested and compared with regular grids and sampling. We asses the numerical prerequisites for all of the above.

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1 Introduction

Feynman path integral (PI) approach offers an intuitively welcome description of non-relativistic quantum mechanics [1, 2], where classical mechanics emerges transparently from disappearing wave nature of particles along with vanishing Planck constant. In PI approach the presentation of the quantum dynamics with a propagator also in stationary quantum states is transparent, in contrast with the conventional approaches, where time evolution is seen in the phase factor, only. However, working out analytical or computational solutions to practical problems becomes more demanding with PI [3, 4], and obviously, this is one of the main reasons for path integrals not being a popular choice for considering quantum dynamics, not to mention the stationary quantum states.

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For the above reasons the dynamical phenomena in nonrelativistic quantum mechanics are conventionally considered by searching or simulating solutions to the time dependent Schrödinger equation. This is almost trivial for a single particle, but becomes laborious and needs a number of approximations with growing complexity in a many-body system. In contrast, with PI the many-body interactions are included transparently and exactly within numerical accuracy. Often, the PI approach is implemented with a stochastic sampling of paths or by analytical formulations like the Kleinert's variational perturbation theory [5].

Out of other approaches than the present, it is worth mentioning the path integral Monte Carlo (PIMC), which has proven to be successful in simulations of periodic imaginary time propagation of many-particle systems, which leads to the finite temperature equilibrium statistical physics description of the many-particle system in terms of mixed state density matrix [6, 7]. By treating all particles with the same PIMC approach it is possible to evaluate the finite temperature electronic structure with exact account of many-body effects and beyond Born–Oppenheimer approximation as demonstrated, already [8,9]. PIMC is also robust enough to be used in various applications in nanoscience [10, 11].

Beyond the analytical solutions to stationary states or quantum dynamics, which are very few [3, 4, 12, 13], numerical simulation of coherent real time propagation faces substantial challenges related to the interference of paths: how to choose or sample the relevant paths in a balanced way, *i.e.* weighting the ones with most contribution through constructive interference and avoiding waste of efforts to those with negligible contribution due to destructive interference. In practice, time evolution of the complex many-body wave function in a space with high number of dimensions leads to even higher dimensional path integrals, which obviously can be sampled efficiently with the Monte Carlo technique, only. There, the interference related slow convergence has been called as "numerical sign problem" [12, 13] or phase (sign) problem. Sophisticated "stationary phase weighting" methods have been developed to overcome this without Monte Carlo technique [14, 15].

There are still no preferable solutions to these problems, although many approaches and approximations for certain types of systems have been found [16, 17]. Basically these methods rely on effective propagators [18] with desired properties. They are relatively well behaving and use the advantageous features of the PI formalism, *e.g.*, reduction of the total system into two parts: the lower dimensional system of interest and the effect of an environment modeled with an influence functional [1]. Often, the effect of the environment can be approximated classically, leaving only a lower dimensional system to be inspected quantum mechanically. Such methods have been shown to be successful in evaluation of the time evolution of a quantum-classical many-body systems [19] for heavier particles than electrons.

Since there is no perfect method for solving dynamical full quantum many-body problems in practice, it is useful to look at different methods, how they can be used, what are their strengths and weaknesses and what is needed in implementation of those