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Real-Time Diffusion Monte Carlo Method

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Abstract. Direct sampling of multi-dimensional systems with quantum Monte Carlo methods allows exact account of many-body effects or particle correlations. The most straightforward approach to solve the Schrödinger equation, Diffusion Monte Carlo, has been used in several benchmark cases for other methods to pursue. Its robustness is based on direct sampling of a positive probability density for diffusion in imaginary time. It has been argued that the corresponding real time diffusion can not be realised, because the corresponding oscillating complex valued distribution can not be used to drive diffusion. Here, we demonstrate that this can be done by turning the distribution piecewise positive and normalisable, and also, by using four types of walkers. This study is a proof of concept demonstration using the well-known and transparent case: one-dimensional harmonic oscillator. Furthermore, we show that our novel method can be used to find not only the ground state but also excited states and even the time evolution of a given wave function. Considering fermionic systems, this method may turn out to be feasible for finding the wave function nodes for other approaches.

AMS subject classifications: 81-08

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1 Introduction

Quantum Monte Carlo (QMC) methods form a collection of robust approaches to study quantum many-particle systems [1]. With QMC the central benefit is that one can deal with multi-dimensional systems, where standard grid based methods become computationally too heavy. With Path Integral and Green's function approaches the many-body effects or correlations can be taken into account without introducing approximations and evaluated within numerical accuracy, which is limited by the computational resources, only. Furthermore, if starting from the first-principles, also the systematic errors are avoidable. Thus, for the field of electronic structure calculations, with QMC one can

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benchmark the energetics and structure of atoms and molecules with desired accuracy. It is even straightforward in cases where the wave function is everywhere positive or can be considered as piecewise positive between given nodes.

Diffusion Monte Carlo (DMC) or Green's function Monte Carlo is a typical representative of QMC. In several cases it has been demonstrated to be a simple but accurate approach to find the ground state [1,2]. In particular, both bosonic [3] and fermionic [4,5] systems have been successfully considered. A recent example is benchmarking the hydrogen molecule and its simple reaction conformations with increasing accuracy [6].

With DMC the Schrödinger equation in imaginary time turns to a diffusion equation, whose "imaginary time evolution" or iteration converges to the ground state. Transformation of the Schrödinger equation to the corresponding integral equation shows how diffusion can be simulated with random walkers guided by the interactions of quantum particles. The walker distribution, which is everywhere positive converges to the ground state wave function. This is the simple idea of DMC simulation, where it is essential that the product of the wave function and diffusion probability is everywhere positive. The latter one is the kernel of the integral equation [6–9].

Due to the everywhere positive "diffusion distribution" interpretation as the wave function, simulation of excited states and indistinguishable fermions becomes problematic with DMC [4,10]. Nodes of the wave function should be known, *e.g.* by symmetry, or approximated with good enough accuracy to make it piecewise positive. Though there are practical approximate ways around the problem, mostly with approximate nodes, this remains as an impediment with DMC.

Based on the probability interpretation of the kernel and wave function, and diffusion nature of the random walk, it has been argued that the simple and useful principles of DMC, above, can not be used to solve the Schrödinger equation with real time path integrals [11, 12]. In this study we show that this is not true and we present a practical solution to this problem, which is related to the sc. "numerical sign problem" of real-time path integrals [12]. Furthermore, we demonstrate that our new real-time path integral approach is capable of finding, not only the ground state, but also excited states, and also, it can be used to simulate proper real time quantum dynamics – not to be mixed with diffusion.

This study is a proof-of-concept demonstration of a novel "real-time DMC". Therefore, we have chosen a transparent test case, the well-known one-dimensional harmonic oscillator (ODHO), where the method and its performance are clearly seen. We also benefit from the exact propagator of the harmonic oscillator while testing the real-time diffusion.

2 Diffusion Monte Carlo and its real time counterpart

2.1 Positive probability density

The well-known imaginary time $(\tau = it)$ integral equation of the conventional Diffusion Monte Carlo (DMC or τDMC) for the many-body wave function ψ is