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Real-time Feynman path integral with Picard–Lefschetz theory and its applications to quantum tunneling

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HIGHLIGHTS

- Real-time path integral is studied based on Picard–Lefschetz theory.
- Lucid demonstration is given through simple examples of quantum mechanics.
- This technique is applied to quantum mechanics of the double-well potential.
- Difficulty for practical applications is revealed, and we discuss its generality.
- Quantum tunneling is shown to be closely related to complex classical solutions.

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ABSTRACT

Picard–Lefschetz theory is applied to path integrals of quantum mechanics, in order to compute real-time dynamics directly. After discussing basic properties of real-time path integrals on Lefschetz thimbles, we demonstrate its computational method in a concrete way by solving three simple examples of quantum mechanics. It is applied to quantum mechanics of a double-well potential, and quantum tunneling is discussed. We identify all of the complex saddle points of the classical action, and their properties are discussed in detail. However a big theoretical difficulty turns out to appear in rewriting the original path integral into a sum of path integrals on Lefschetz thimbles. We discuss generality of that problem and mention its importance. Real-time tunneling processes are shown to be described by those complex saddle points, and thus semi-classical description of real-time quantum

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tunneling becomes possible on solid ground if we could solve that problem.

1. Introduction

Quantum real-time dynamics has been an important topic for vast areas of physics, especially related to nonequilibrium phenomena. Since quantum mechanics deals superposition of probability amplitudes, the Feynman path integral says that time-development of quantum states can be viewed as a sum of amplitudes $\exp(\mathrm{i}S[x(t)]/\hbar)$ over all possible spacetime paths $x(t)$ [1,2]. However, such summations show truly bad convergence due to the highly oscillatory factor without any suppressions. This leads to non-existence of the real-time path integral as the standard integration theory [3], and also makes difficult its numerical simulation due to the severe sign problem. From measure theoretical point of view, its close relation to the Wiener integration is first revealed by Kac when time t is replaced by the imaginary time $-\mathrm{i}\tau$ [4] (see also Refs. [5,6]). Imaginary-time path integral provides a convenient formalism also for numerical computations for thermal equilibrium systems, but analytic continuation must be performed to obtain real-time dynamics. Realization of real-time path integrals based on the measure theory itself is an interesting task in mathematical physics, but it will also provide a convenient framework for direct simulations of quantum real-time phenomena.

Recently, Witten proposed an application of Picard–Lefschetz theory to Feynman path integral [7,8]. Picard–Lefschetz theory, which is a complex analogue of Morse theory, tells us all possible deformations of an integration contour in the complexified space of an original integration cycle. Therefore, we are free from oscillatory integrals by choosing "nice" integration cycles, which are called Lefschetz thimbles. This technique has a potential to reveal nonperturbative aspects of quantum field theory. Indeed, there is already an interesting suggestion that existence of Lefschetz thimbles around nonperturbative critical points may be closely related to ambiguities of Borel summation of perturbation theory [9–11]. Its practical applications are now also being studied especially for solving the sign problem in Monte Carlo simulations of statistical quantum systems; finite-density quantum chromodynamics [12–16], and repulsive Hubbard model in condensed matter physics [17].

In this paper, Picard–Lefschetz theory is applied to real-time path integrals of quantum systems. After reviewing the path-integral formalism based on Picard–Lefschetz theory, we first study fundamental properties of path integrals on Lefschetz thimbles. In order to show how this method works, simple examples of quantum mechanics are considered, and Feynman kernels are computed for free particles and for a harmonic oscillator by using path integrals on Lefschetz thimbles. We will be able to see at least for these examples that real-time path integrals are now well-defined based on the standard integration theory on Lefschetz thimbles.

As an application of this formalism, quantum mechanics of a double-well potential is considered, and quantum tunneling is discussed. We identify all saddle points of the classical action in the complexified space of spacetime paths, and their properties are discussed in detail. However a big theoretical difficulty turns out to appear in rewriting the original path integral into a sum of path integrals on Lefschetz thimbles. We discuss generality of that problem and mention its importance for future numerical computations of path integrals with sign problem. We do not solve this problem in a direct way, but we argue that real-time tunneling must be described by highly-oscillatory complex classical solutions, by scrutinizing those solutions both in real-time and imaginary-time formalisms. Therefore, we can obtain exact semi-classical description of real-time quantum tunneling on solid ground if we could solve that theoretical difficulty.

This paper is organized as follows. In Section 2, we first briefly review applications of Picard–Lefschetz theory to path integrals. After that, we discuss basic properties of path integrals on each Lefschetz thimble. In Section 3, we demonstrate how to compute real-time path integrals