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Complex saddle points and the sign problem in complex Langevin simulation

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Abstract

We show that complex Langevin simulation converges to a wrong result within the semiclassical analysis, by relating it to the Lefschetz-thimble path integral, when the path-integral weight has different phases among dominant complex saddle points. Equilibrium solution of the complex Langevin equation forms local distributions around complex saddle points. Its ensemble average approximately becomes a direct sum of the average in each local distribution, where relative phases among them are dropped. We propose that by taking these phases into account through reweighting, we can solve the wrong convergence problem. However, this prescription may lead to a recurrence of the sign problem in the complex Langevin method for quantum many-body systems.

1. Introduction

Precise analysis of thermodynamic properties of a quantum many-body system, in particular, precise determination of its phase diagram is one of great challenges in theoretical physics. An *ab initio* simulation based on lattice field theory, in particular, so called Monte Carlo simulation is the most powerful tool for this. In many interesting cases, however, Monte Carlo simula-

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tion is hindered by the notorious sign problem. The importance sampling, using the Boltzmann weight e^{-S}, breaks down when the action becomes complex. In hadron physics, lattice quantum chromodynamics (QCD) simulation suffers from the sign problem at finite quark densities [1,2], which is important to study quark matter inside neutron stars [3,4]. The sign problem occurs also in condensed matter systems [5–7]. Important examples are the fermionic Hubbard model away from half-filling, and geometric frustration in spin systems. A method to overcome the sign problem attracts a broad interest for application to the aforedescribed quantum many-body systems.

There have been a lot of attempts to tackle the sign problem. Among them, idea of complexification of the integration variables is one promising way to solve the sign problem. Theoretical attempts along this line are classified into two approaches, that is, the Lefschetz-thimble and the complex Langevin methods. The Picard–Lefschetz theory gives a generalization of the steepest descent method, and Lefschetz thimbles are steepest descent paths in the extended complex plane [8–10]. This method is formulated on rigorous mathematics, but it needs some approximation when applied to quantum many-body systems [11–16]. On the other hand, the complex Langevin method is an extension of the Langevin equation to a complex Boltzmann weight [17–20]. The numerical implementation of this is possible based on lattice field theory. The complex Langevin method has been widely applied from condensed matter to hadron physics [21–26]. There is a formal proof [27,28] on the correctness of the complex Langevin method, where it has been shown that the complex Langevin method correctly gives physical observables if the distribution obtained from the Langevin equation damps exponentially fast around infinities and singular points. This method is, however, known to give wrong results for some cases, where distribution does not show the exponentially fast decay, and thus the formal proof cannot be applied (for recent discussions, see also [29–35]). Therefore, it is important to unveil what properties of the classical action cause the wrong convergence of the complex Langevin method.

In this paper, we show within the semiclassical analysis that complex Langevin simulation converges to a wrong result, when path-integral weight at complex saddle points has different phases. This includes the case of the breakdown due to a singular drift term, e.g., the lattice QCD at finite density. We reveal that complex Langevin simulation breaks down more generic case where the Langevin drift term has no singular point. With the help of semiclassical analysis, we find that reweighting by the complex phase can partially solve the wrong convergence problem. However, the reweighting leads, in general, to a severe cancellation of the reweighting factor in many-body systems, which is nothing but a sign problem in terms of the complex Langevin method.

2. Complex Langevin method and its failure

For simplicity, we discuss an oscillatory integral of one variable x, which can be extended to multiple integrals in a straightforward way,

$$\langle O(x)\rangle = \frac{1}{Z}\int_{\mathbb{R}} \mathrm{d}x\, e^{-S(x)/\hbar} O(x), \tag{1}$$

where Z is the normalization factor. The action $S(x)$ is complex valued in general, which makes the Monte Carlo simulation of Eq. (1) difficult because of the sign problem. One proposal to calculate Eq. (1) for a complex valued action is the so-called complex Langevin method [18–20].