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Non-renormalizability of the HMC algorithm

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Abstract:

In lattice field theory, renormalizable simulation algorithms are attractive, because their scaling behaviour as a function of the lattice spacing is predictable. Algorithms implementing the Langevin equation, for example, are known to be renormalizable if the simulated theory is. In this paper we show that the situation is different in the case of the molecular-dynamics evolution on which the HMC algorithm is based. More precisely, studying the φ 4 theory, we find that the hyperbolic character of the molecular-dynamics equations leads to non-local (and thus non-removable) ultraviolet singularities already at one-loop order of perturbation theory.

Keywords: Lattice QCD, Lattice Quantum Field Theory, Renormalization Regularization and Renormalons.

Introduction

Numerical simulations in lattice field theory are based on stochastic processes that produce random sequences of representative field configurations. It is often useful to interpret the simulation time in these calculations as a further space-time coordinate. The n-point autocorrelation functions of the local fields then formally look like the correlation functions in a field theory with an extra dimension and they are, in fact, sometimes representable in this way. Depending on the simulation algorithm, and if the simulated theory is renormalizable, the autocorrelation functions may conceivably be renormalizable as well. The scaling properties of such algorithms (which, for brevity, will be referred to as renormalizable) are encoded in the continuum theory and thus become predictable to some extent.

In the pure SU(N) gauge theory, for example, simulation algorithms that integrate the Langevin equation are known to be renormalizable [1, 2]. The integrated autocorrelation times τint of physical observables have dimension [length]2 in this case. Moreover, the standard renormalization group analysis and a one-loop calculation in

perturbation theory [3–5] imply that they scale according to [6]

$$\tau_{\rm int} = C g_0^{9/11} \left\{1 + \mathrm{O}(g_0^2)\right\} r_0^2$$

at small lattice spacings a, where C is an observable-dependent constant, g0 the bare gauge coupling and r0 the Sommer radius [11]. In lattice units, the autocorrelation times thus increase like 1/a2 as a → 0 up to a logarithmically decreasing factor.1

Most simulations of lattice QCD performed today are based on some variant of the HMC algorithm [12]. The form of the underlying molecular-dynamics equations and freefield studies [13] suggest that the simulation time has physical dimension [length] in this case and that the autocorrelation times consequently scale essentially like 1/a. As far we know, the renormalizability of the algorithm has however never been studied and its scaling properties in presence of interactions thus remain unknown.

In this paper, the issue is addressed in the framework of perturbation theory. For simplicity

the φ 4 theory is considered, but our main result (the non-renormalizability of the molecular-dynamics equations) no doubt extends to most theories of interest. A slightly generalized version of the HMC algorithm is studied, which was introduced many years ago by Horowitz [14–16] (see sections 2 and 3). The non-renormalizability of the associated stochastic equation is then established by showing that the four-point autocorrelation function of the fundamental field has a non-removable ultraviolet singularity at second order in the coupling (sections 4 and 5).

Stochastic molecular dynamics

In order to simplify the discussion as much as possible, we consider the φ 4 theory with a single scalar field φ and dimensional instead of a lattice regularization. The action of the field in D = 4 − 2ϱ Euclidean dimensions is given by where m0 denotes the bare mass parameter and g0 the bare coupling constant. The generalized HMC algorithm [14–16] integrates a stochastic version of the molecular-dynamics equations that derive from the action (2.1). In the following subsections, we briefly discuss these equations and solve them in powers of the coupling g0.

$$S = \int \mathrm{d}^D x \left\{ \frac{1}{2}\partial_\mu\phi(x)\partial_\mu\phi(x) + \frac{1}{2}m_0^2\phi(x)^2 + \frac{g}{4}\right.$$

Evolution equations

As usual the molecular dynamics evolves the field φ(t, x) together with its momentum π(t, x) as a function of a fictitious time t. The stochastic evolution equations [14–16]

$$\begin{aligned}\partial_t\phi &= \pi,\\ \partial_t\pi &= -\frac{\delta S}{\delta\phi} - 2\mu_0\pi + \eta\\ &= (\partial_\mu\partial_\mu - m_0^2)\phi - \frac{g_0}{3!}\phi^3 - 2\mu_0\pi + \eta,\end{aligned}$$

involve another mass parameter, μ0 > 0, and a Gaussian noise η(t, x) with vanishing expectation value and variance.

$$\langle\eta(t,x)\eta(s,y)\rangle = 4\mu_0\delta(t-s)\delta(x-y).$$

Evidently, the ordinary molecular dynamics is recovered in the limit μ0 → 0. Moreover, in the second-order form,

$$\partial_t^2\phi + 2\mu_0\partial_t\phi = -\frac{\delta S}{\delta\phi} + \eta,$$

and after substituting t → 2μ0t, the evolution equations are seen to coincide with the Langevin equation up to a term that goes to zero at large μ0.

Since its introduction by Horowitz [14–16], the generalized HMC algorithm has been occasionally studied in the literature, where it is referred to as the Kramers equation or the L2MC algorithm (see refs. [13, 17, 18], for example). In practice, one starts from the firstorder equations (2.2), (2.3) and implements the algorithm using symplectic integrators and acceptance-rejection steps. For the theoretical analysis in this paper, we however prefer to proceed with the second-order equation (2.5).

Relation to the ordinary correlation functions

Since the stochastic molecular dynamics simulates the field theory with action (2.1), the equal-time autocorrelation functions

$$\tilde{C}_n(p_1,\ldots,p_n) = \int_{\omega_1\ldots\omega_n} \tilde{A}_n(\omega_1,p_1;\ldots;\omega_n,p_n)$$

must coincide with the ordinary correlation functions of the fundamental field in momentum space [14–16]. In this section, we show that the two- and the four-point autocorrelation functions do have this property at one-loop order of perturbation theory. Partly the calculation serves as a consistency check, but some of the intermediate results will be helpful in section 5 as well, where we discuss the non-renormalizability of the stochastic molecular dynamics.

Concluding remarks

The HMC algorithm is currently the preferred simulation algorithm in lattice QCD. In the past two decades, various improvements were included in this algorithm, many of them with the aim of reducing the computational effort required at small sea-quark masses (see ref. [20] for a recent review). Its scaling behaviour with respect to the lattice spacing has not received as much attention so far, but rapidly becomes an important issue when the continuum limit is approached.

While the dynamical properties of the HMC algorithm are well understood in free field theory [13], the situation in the presence of interactions tends to be rather more complicated. In particular, certain lattice artifacts (topology-changing tunneling transitions, for example, or unphysical critical points in the space of bare couplings) can cause large autocorrelations. The results obtained in this paper show that even in the absence of such effects there is no reason to expect that the HMC algorithm scales essentially as in a theory of free fields. Evidently, the non-renormalizability of the algorithm does not imply that it is invalid or unusable close to the continuum limit, but without further insight its scaling behaviour is unpredictable in interacting theories.

The HMC algorithm and the stochastic molecular dynamics may conceivably fall into the universality class of the Langevin equation. Independently of whether this is the case or not, it may be worth looking for renormalizable algorithms where the simulation time has scaling dimension less than 2. Eventually such algorithms might turn out to be faster than the HMC algorithm and they would have the advantage that their efficiency at small lattice spacings is predictable.

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