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A Study of the Non-Renormalizability in the HMC Algorithm

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Abstract:

Renormalizable simulation methods are appealing in lattice field theory because of their predictable scaling behaviour as a function of the lattice spacing. If the simulated theory is renormalizable, algorithms that implement the Langevin equation, for instance, are known to be renormalizable. In this study, we demonstrate that the molecular-dynamics evolution, on which the HMC algorithm is based, presents a new set of circumstances. More specifically, we discover that, at the perturbation theory's first-loop order, the hyperbolic nature of the molecular-dynamics equations causes non-local (and consequently non-removable) ultraviolet singularities.

Keywords: Lattice QCD, Lattice Quantum Field Theory, Renormalization Regularizeton 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 – 1 – JHEP04(2011)104 way. Depending on the simulation algorithm, and if the simulated theory is renormalizedable, 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 autoscorelotion times hint 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 [

$$\tau_{\text{int}} = C g_0^{9/11} \{1 + O(g_0^2)\} r_0^2 \qquad (1.1)$$

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 simplicate 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-

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renormalizability of the associated stochastic equation is then established by showing that the four-point autocorrelation funkton of the fundamental field has a non-removable ultraviolet singularity at second order in the coupling (sections 4 and 5).

$$S = \int \mathrm{d}^D x \left\{ \frac{1}{2}\partial_\mu \phi(x)\partial_\mu \phi(x) + \frac{1}{2}m_0^2 \phi(x)^2 + \frac{g_0}{4!}\phi(x)^4 \right\}, \tag{2.1}$$

where m0 denotes the bare mass parameter and g0 the bare coupling constant. The genrealized HMC algorithm [14–16] integrates a stochastic version of the molecular-dynamics

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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]

$$\partial_t \phi = \pi, \tag{2.2}$$

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

$$= (\partial_\mu \partial_\mu - m_0^2)\phi - \frac{g_0}{3!}\phi^3 - 2\mu_0 \pi + \eta, \tag{2.3}$$

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

$$\langle \eta(t,x)\eta(s,y)\rangle = 4\mu_0 \delta(t-s)\delta(x-y). \tag{2.4}$$

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

$$\partial_t^2 \phi + 2\mu_0 \partial_t \phi = -\frac{\delta S}{\delta \phi} + \eta, \tag{2.5}$$

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 Kramer's 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 simplistic integrators and acceptance-rejection steps. For the theoretical analysis in this paper, we however

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
prefer to proceed with the second-order equation (2.5).

Solution of eq. (2.5) to leading order in go:

The leading-order equation

$$\mathcal{D}\phi_0 = \eta, \tag{2.6}$$

$$\mathcal{D} = \partial_t^2 + 2\mu_0 \partial_t - \partial_\mu \partial_\mu + m_0^2, \tag{2.7}$$

coincides with the Klein-Gordon equation in D + 1 dimensions except for the term propertonal to μ0, which tends to damp the time evolution of the field. At large μ0 and after a rescaling of t, the equation actually turns into the heat equation. The Green function

$$K(t,x) = \int_{\omega,p} \mathrm{e}^{-i\omega t + ipx} \tilde{K}(\omega,p), \tag{2.8}$$

$$\tilde{K}(\omega,p) = \left(-\omega^2 - 2i\mu_0\omega + p^2 + m_0^2\right)^{-1}, \tag{2.9}$$

of the differential operator D is discussed in some detail in appendix A. Here and below, the notational convention

$$\int_\omega = \int \frac{\mathrm{d}\omega}{2\pi}, \qquad \int_p = \int \frac{\mathrm{d}^D p}{(2\pi)^D}, \tag{2.10}$$

is used. It is then straightforward to show that the solution of the wave equation (2.6) at time t ≥ t0 with prescribed initial data at time t0 is given by

$$\phi_0(t,x) = \int_{t_0}^{t} \mathrm{d}s \int \mathrm{d}^D y\, K(t-s, x-y)\eta(s,y) \tag{2.11}$$

$$+ \int \mathrm{d}^D y \left\{ K(t-t_0, x-y)(\partial_t \phi_0)(t_0,y) + (\partial_t + 2\mu_0)K(t-t_0, x-y)\phi_0(t_0,y) \right\}.$$

Note that the dependence on the initial data dies away exponentially with increasing time (see appendix A). The stochastic molecular-dynamics evolution thus thermalizes and eventally loses all memory of the initial values of the field. In the following, we shall only be interested in the behaviour of the autocorrelation functions after thermalization. We therefore move the thermalization phase to time t0 = −∞ and are then left with the solution

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$$\phi_0(t,x) = \int_{-\infty}^{t} \mathrm{d}s \int \mathrm{d}^D y\, K(t-s, x-y)\eta(s,y) \qquad (2.12)$$

Iterative solution of the evolution equation

Equation (2.5) may be written in the form

$$\mathcal{D}\phi = \eta - \frac{g_0}{3!}\phi^3 \qquad (2.13)$$

or, equivalently, as an integral equation

$$\phi(t,x) = \phi_0(t,x) - \frac{g_0}{3!}\int_{-\infty}^{t} \mathrm{d}s \int \mathrm{d}^D y\, K(t-s, x-y)\phi(s,y)^3. \qquad (2.14)$$

Iteration of the latter then yields the solution $\phi(t,x)$ in powers of g_0.

Each term in this expansion may be represented by a tree diagram with directed lines, four-point and one-point vertices (see figure 1). In frequency-momentum space,

$$\tilde{\phi}(\omega,p) = \int \mathrm{d}t\, \mathrm{d}^D x\, e^{i\omega t - ipx}\phi(t,x), \qquad (2.15)$$

the lines represent the Green function

$$\xleftarrow[\omega,p]{} = \tilde{K}(\omega,p), \qquad (2.16)$$

while the one-point vertices

$$\omega,p \rightarrow \otimes = \tilde{\eta}(\omega,p) \qquad (2.17)$$

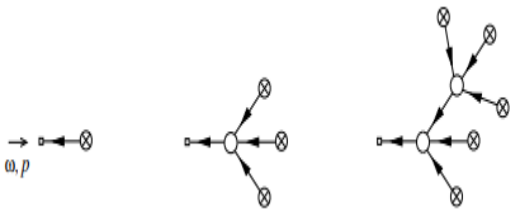

Figure 1. In perturbation theory, the solution of the integral equation (2.14) is given by a series of directed tree diagrams. The diagrams up to second order in g0 are shown in this figure. All diagrams have a single external line (labelled by a little square) with ingoing frequency-momentum (ω, p). The arrows on the internal lines all point in the direction towards the external line. stand for the insertion of the noise field. As in ordinary Feynman diagrams, there is a frequency-momentum conservation δ-function

$$(2\pi)^{D+1}\delta(\omega_1+\omega_2+\omega_3+\omega_4)\delta(p_1+p_2+p_3+p_4) \qquad (2.18)$$

associated to each vertex

$$\oplus = -g_0 \qquad (2.19)$$

with ingoing frequency-momenta (ω1, p1), . . ., (ω4, p4). The lines in these diagrams are directed, because K˜ (ω, p) is not invariant under a change of sign of ω. In position space, the arrows point in the direction of increasing simulation time.

Autocorrelation functions

The n-point autocorrelation functions of the field φ (t, x) are usually defined by taking the time average of the product φ (t1, x1) . . . φ (Tn, an) at fixed time lags it − to. In the present setup, the translation symmetry in time allows the time average to be replaced by the Avenrage h. i over the noise field η (s, y). We are thus led to consider the correlation funk

$$\tilde{A}_n(\omega_1,p_1;\ldots;\omega_n,p_n) = \langle\tilde{\phi}(\omega_1,p_1)\ldots\tilde{\phi}(\omega_n,p_n)\rangle \qquad (3.1)$$

in frequency-momentum space, which may be computed in perturbation theory by ex-pending the fields φ˜ (wk., pk) in powers of the coupling g0, following the lines of the previous section, and by contracting the noise fields using Wick's rule. As a result, one obtains a sum of Feynman diagrams for the autocorrelation functions similar to the ones for the ordinary (field-theoretical) correlation functions.

Feynman rules:

The one-point vertices in the tree diagrams that represent the terms in the expansion of φ˜ (wk., pk) are connected to the rest of the tree through a directed line. When the noise fields at any two such vertices are contracted, an undirected line

Non-renormalizability of the stochastic molecular dynamics:

We now address the question whether the ultraviolet singularities of the autocorrelation functions can be cancelled by the addition of local counter terms to the evolution equalton (2.5).

Parameter renormalization

Evidently, the list of counter terms must include those corresponding to the usual parameter and field renormalization that is required for the renormalization of the ordinary correlation functions. In the minimal subtraction scheme, the bare coupling and mass are related to the renormalized parameters g and m through

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$$g_0 = M^{2\epsilon} g \left\{ 1 + \frac{3g}{32\pi^2 \epsilon} + O(g^2) \right\}, \tag{5.1}$$

$$m_0^2 = m^2 \left\{ 1 + \frac{g}{32\pi^2 \epsilon} + O(g^2) \right\}, \tag{5.2}$$

where M denotes the normalization mass. To one-loop order, the fundamental field does not need to be renormalized in this theory. Recalling east. (4.2), (4.8) and (4.9), it is then immediately clear that the parameter renormalization cancels the singularities of the two- and four-point autocorrelation funktons which derive from the poles (3.8) and (3.16) of the integrals I1 and

Non-renormalizability of the four-point function

The four-point autocorrelation function has further singularities proportional to the diverging part (3.18) of the integral J1. As explained in section 4, the ordinary four-point correlation function does not receive any contributions from this integral (and is therefore finite after the parameter renormalization), but the terms proportional to J1 do contribute to the autocorrelation function at non-zero-time separations. The residue of the pole in eq. (3.18) is the Fourier transform of a distribution

$$\frac{e^{-2\mu_0 t}}{32\pi^4 x^2} \theta(t) \delta(t^2 - x^2) \tag{5.3}$$

supported on the light cone t = |x|. Both diagrams 2 and 3 thus have a non-local singlaity that cannot be cancelled by including local counter terms in the stochastic molecular dynamics. The latter is therefore not renormalizable. The presence of the singularity (5.3) can be understood by noting that the integrand of the integral

$$J_1(\omega, p) = \int_0^\infty dt \int d^D x \, e^{i\omega t - ipx} G(t, x)^2 \tag{5.4}$$

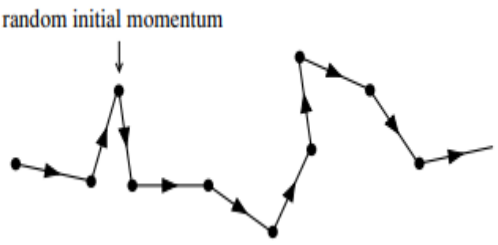

Figure 3. The HMC algorithm moves the fundamental field φ through field space along a piecewise smooth curve. In the smooth segments of the curve, the field is evolved from time t = 0 to sometime t = τ according to the molecular-dynamics equations, starting from the current field φ and Gaussian random values for its momentum π. has a non-integrable singularity in D = 4 dimensions proportional to (t − |x|) −1 (see subsection A.3). Such light-cone singularities are a characteristic feature of green functions of hyperbolic wave equations and the non-renormalizability of the stochastic molecular dynamics is thus seen to be related to its hyperbolic nature. In ordinary field theory, one-loop integrals do not have non-local ultraviolet singlaities, because they can be Wick rotated to Euclidean space where the propagators are singular at coinciding points only. The spectral condition and the locality of the theory guarantee that no singularities stand in the way of the Wick rotation [19]. In the case of the diagrams 2 and 3, however, the integrands have poles in all quadrants of the complex frequency plane and the integrals (3.9) and (3.10) consequently cannot be Wick rotated without generating additional terms.

Implications for the HMC algorithm:

In practice, the HMC algorithm involves a numerical integration of the (ordinary) molecular-dynamics equations and acceptance-rejection steps to correct for the integration errors. For simplicity the integration is assumed to be exact in this section. No acceptancerejection steps are then required and whether one uses the first- or the second-order form of the molecular-dynamics equations makes no difference. The molecular-dynamics trajectories generated by the algorithm are smooth segments of a continuous curve in field space (see figure 3). Along the trajectories, the n-point autocorrelation functions in the time-momentum representation,

$$\hat{A}_n(t_1, p_1; \ldots; t_n, p_n) = \langle \hat{\phi}(t_1, p_1) \ldots \hat{\phi}(t_n, p_n) \rangle, \qquad 0 \le t_k \le \tau, \tag{5.5}$$

may be defined, where the bracket h. i stands for the average over all trajectories in an infinitely long simulation. The autocorrelation functions (5.5) only describe the dynamical properties of the algorithm in the specified range of times, but the discussion in the following paragraphs shows that already these correlation functions are not renormalizable. The average over trajectories in eq. (5.5) amounts to taking the average over the initial values of the field φ and its momentum π = ∂to. Since these are distributed according to the equilibrium distribution (a Gaussian in the case of the momentum), the average coincides with the ordinary expectation value. In perturbation theory, the correlation – 12 – JHEP04(2011)104 functions can therefore be calculated by solving the (non-stochastic) molecular-dynamics equations in the range 0 ≤ t ≤ τ with prescribed initial data at t = 0 and by

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computing the expectation value of the product φˆ (t1, p1) . . . φˆ (Tn, pan) using the standard Feynman rules for the correlation functions of the initial data. In the case of the stochastic molecular dynamics, the computation of the autoscorelotion functions in the time-momentum representation can be organized in the same way. A notable difference is that the contractions of the noise field give rise to additional digrams, but since all these diagrams disappear in the limit μ0 → 0, it is clear that the autocorrelation functions (5.5) are given by

$$\hat{A}_n(t_1,p_1;\ldots;t_n,p_n)=\lim_{\mu_0\downarrow 0}\int_{\omega_1,\ldots,\omega_n} e^{-i(\omega_1 t_1+\cdots+\omega_n t_n)}\tilde{A}_n(\omega_1,p_1;\ldots;\omega_n,p_n), \qquad (5.6)$$

where the autocorrelation functions on the right are those discussed in the previous sections. Note that the frequency integrals must be performed before μ0 is taken to zero, as otherwise one may run into infrared-singular intermediate expressions. In view of its relation to the stochastic molecular dynamics, as expressed through eq. (5.6), and since the distribution (5.3) remains non-local at μ0 = 0, we are thus led to conclude that also the HMC algorithm is not renormalizable.

The Langevin limit:

As already mentioned in subsection 2.1, the stochastic molecular-dynamics equation (2.5) is equivalent to the Langevin equation in the limit μ0 → ∞ up to a rescaling of the simulation time.2 The associated n-point autocorrelation functions

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 tunnelling 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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