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Numerical Stochastic Perturbation Theory and Gradient Flow in φ^4 Theory

Mattia Dalla Brida
NIC, DESY, Platanenallee 6, 15738 Zeuthen, Germany
E-mail: mattia.dalla.brida@desy.de

Marco Garofalo*
Higgs Centre for Theoretical Physics, School of Physics and Astronomy,
The University of Edinburgh, Edinburgh EH9 3JZ, Scotland, UK
E-mail: M.Garofalo@sms.ed.ac.uk

Anthony D. Kennedy
Higgs Centre for Theoretical Physics, School of Physics and Astronomy,
The University of Edinburgh, Edinburgh EH9 3JZ, Scotland, UK
E-mail: adk@ph.ed.ac.uk

In this contribution we present an exploratory study of several novel methods for numerical stochastic perturbation theory. For the investigation we consider observables defined through the gradient flow in the simple φ^4 theory.

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*Speaker.

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1. Introduction

The information from lattice perturbation theory (LPT) can be valuable for non-perturbative investigations of lattice field theories. For instance LPT allows the matching of renormalization schemes at high-energy to be determined, and it can provide useful insights on the lattice artifacts of the observables of interest. As well known, LPT is made more difficult than its continuum counterpart by the complicated expressions for vertices and propagators that normally force numerical evaluation even for simple diagrams. Additionally, in the case of gauge theories the appearance of new vertices at all orders of perturbation theory makes the number of diagrams grow rapidly with the perturbative order, thus leaving only low-order results accessible to standard techniques. Numerical stochastic perturbation theory (NSPT) was introduced some time ago [1] (see [2, 3] for recent developments) in order to bypass these difficulties, and thus allow estimates of high-order perturbative coefficients to be obtained. The basic idea of NSPT is to integrate numerically a discrete version of the equations of stochastic perturbation theory. The method comes with two main limitations: first of all it is not exact, a sequence of simulations with a finer and finer discretization of the relevant equations have to be performed in order to extrapolate away the systematic errors in the results, secondly, the numerical simulations suffer from critical slowing down as the continuum limit of the theory is approached.

Martin Lüscher has recently proposed a new form of stochastic perturbation theory, namely Instantaneous Stochastic Perturbation Theory (ISPT) [4], which completely eliminates these limitations; this contribution presents an exploratory study of this technique. Moreover, we propose new NSPT methods using stochastic equations other than the Langevin equation. As we shall see this leads to more efficient numerical algorithms that can significantly alleviate the limitations of the standard set-up. For simplicity we test these methods in a simple scalar φ^4 theory defined on a finite Euclidean 4-dimensional periodic lattice of size L with action given by,

$$S(\varphi) = \sum_x \left\{ \frac{1}{2}\partial_\mu \varphi(x)\partial_\mu \varphi(x) + \frac{1}{2}m_0^2\varphi(x)^2 + \frac{g_0}{4!}\varphi(x)^4 \right\}. \tag{1.1}$$

Here $\partial_\mu \varphi(x) = [\varphi(x+a\hat{\mu}) - \varphi(x)]/a$, with $\mu = 0,\ldots,3$ defines the usual forward lattice derivative where $\hat{\mu}$ is the unit vector in the direction μ and a is the lattice spacing. The parameters m_0 and g_0 are the bare mass and coupling, respectively.

2. ISPT

ISPT is based on the concept of trivializing maps [4]. These transform Gaussian distributed fields $\eta_i(x)$ into a stochastic field $\phi(x)$ such that,

$$\langle \phi(x_1)...\phi(x_n)\rangle_\eta = \langle \varphi(x_1)...\varphi(x_n)\rangle, \tag{2.1}$$

where φ is the field with action (1.1), $\langle\cdots\rangle$ is the expectation value in the φ^4 theory, and $\langle\cdots\rangle_\eta$ denotes the average over the fields $\eta_i(x)$ which satisfy

$$\langle \eta_i(x)\eta_j(y)\rangle_\eta = \delta_{ij}\,\delta_{xy}, \qquad \langle \eta_i(x)\rangle_\eta = 0. \tag{2.2}$$

Without entering into the details (for which we refer to [4]), the stochastic field $\phi(x)$ can be written as a power series in the couplings of the theory, whose coefficients are calculable functions of the

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noise fields $\eta_i(x)$. For φ^4 theory

$$\phi(x) = \sum_{j,k=0}^{\infty} \phi_{(j,k)}(x)(\delta m^2)^j g_0^k, \tag{2.3}$$

where the coefficients $\phi_{(j,k)}(x)$ depend on the values of the noise fields $\eta_i(x)$. Note that the expansion is in terms of the bare coupling g_0, and the mass counterterm $\delta m^2 = m_0^2 - m^2$, where m is the renormalized mass. This method generates uncorrelated field configurations, unlike methods based on Markov processes (see below), and it is exact in the sense that the only source of uncertainly in the results comes from the stochastic evaluation of the Gaussian integrals in (2.1). Being a diagrammatic technique, however, the number of contributions and thus the cost of evaluating the coefficients $\phi_{(j,k)}$ grows rapidly with the perturbative order [4].

For this work we wrote a code for the automated computation of the trivializing map ϕ in the φ^4 theory to arbitrary order in the couplings.[1] As a test of our implementation we computed the finite-volume coupling defined in [5] for several lattice volumes and mass values, and compared the results with their analytic perturbative expansion up to three-loop order. We found excellent agreement within the per-mill precision we reached.

3. LSPT

The original way to implement numerical stochastic perturbation theory [1] is to generate the stochastic field $\phi(x)$ via a Markov process based on the Langevin equation (LSPT),

$$\partial_{t_s}\phi(x,t_s) = \partial^2\phi(x,t_s) - (m^2+\delta m^2)\phi(x,t_s) - \frac{g_0}{3!}\phi(x,t_s)^3 + \eta(x,t_s), \tag{3.1}$$

where t_s is the simulation time, ∂^2 the lattice Laplacian, and $\eta(x,t_s)$ is a Gaussian distributed noise field satisfying $\langle\eta(x,t_s)\rangle_\eta = 0$ and $\langle\eta(x,t_s)\eta(y,t_s')\rangle_\eta = 2\delta_{xy}\delta(t_s - t_s')$. As in ISPT, the field $\phi(x,t_s)$ is assumed to have an expansion of the form (2.3), while the noise $\eta(x,t_s)$ only has a lowest order component. The expectation values of the target theory are then obtained as,

$$\langle\phi(x_1,t_s)...\phi(x_n,t_s)\rangle_\eta \overset{t_s\to\infty}{=} \langle\varphi(x_1)...\varphi(x_n)\rangle. \tag{3.2}$$

The way one proceeds is to discretize the stochastic time as $t_s = n\varepsilon$, with ε the step-size, and integrate the Langevin equations numerically order-by-order in couplings g_0 and δm^2 according to a given integration scheme. Consequently, one expects step-size errors to effect the results, which thus need to be extrapolated away. Moreover, the fields $\phi(x,t_s)$ generated in this way are correlated to each other. On the other hand, the cost of the method scales only quadratically with the perturbative orders in the couplings.

4. HSPT

Taking inspiration from the Langevin approach, we also considered whether using different stochastic differential equations might improve LSPT.

[1] For the construction of the trivializing map we used the publicly available code provided by Martin Lüscher at `luscher.web.cern.ch/luscher/ISPT`.

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One possibility is to use the Hybrid Molecular Dynamics equations (HSPT),

$$\partial_{t_s}\phi(x,t_s)=\pi(x,t_s),\qquad \partial_{t_s}\pi(x,t_s)=\partial^2\phi(x,t_s)-(m^2+\delta m^2)\phi(x,t_s)-\frac{g_0}{3!}\phi(x,t_s)^3. \tag{4.1}$$

Here the momentum field $\pi(x,t_s)$ is also considered as a series (2.3) in the couplings, and it is sampled from a Gaussian distribution $P(\pi)\propto e^{-\frac{\pi^2}{2}}$ at the beginning of each trajectory. In particular, at the start of each trajectory the momenta only have a non-zero lowest order component, while they acquire higher-order components through the MD evolution. As in the Langevin case, the simulation time needs to be discretized, $t_s=n\delta t$, and the MD equations integrated numerically order-by-order in g_0 and δm^2 up to a time $t_s=\tau$ according to some integrator. Expectation values in the target theory are then similarly obtained as in (3.2) by averaging over the trajectories [6]. In order to have an ergodic algorithm, one needs to randomize the trajectory lengths τ so to update all frequency components of the field ϕ, including the ones of the lowest order field $\phi_{(0,0)}$ [7].

5. KSPT

Another possibility that is worth exploring is to generate the field $\phi(x)$ through a stochastic evolution in phase-space according to Kramers equations [8] (see also [6]) (KSPT),

$$\begin{aligned}&\partial_{t_s}\phi(x,t_s)=\pi(x,t_s),\\&\partial_{t_s}\pi(x,t_s)=-\gamma\pi(x,t_s)+\partial^2\phi(x,t_s)-(m^2+\delta m^2)\phi(x,t_s)-\frac{g_0}{3!}\phi(x,t_s)^3+\eta(x,t_s).\end{aligned} \tag{5.1}$$

The corresponding algorithm is obtained by alternating a partial refreshment of the momentum field, $\pi'=e^{-\gamma\delta t}\pi+\sqrt{1-e^{-2\gamma\delta t}}\eta$, with the numerical integration of the MD equations for a time-step, using a suitable integrator. Here $\eta(x,t_s)$ is a Gaussian noise field with zero mean and variance $\langle\eta(x,t_s)\eta(y,t_s')\rangle=\delta_{xy}\delta(t_s-t_s')$, while γ is a free parameter that may be tuned to minimize auto-correlations. As in the Langevin case, the noise field only has a lowest order component, while the fields ϕ and π have an expansion of the form (2.3). For $\gamma=0$ the algorithm reduces to a single-step HSPT with trajectory length $\tau=\delta t$. On the contrary, if the continuum limit of the theory is taken keeping the parameter γ fixed in lattice units, the equations (5.1) can be shown to reduce to the Langevin equation (3.1) [6].

6. Observables

In order to test the different methods we rely on observables defined through the gradient flow [9]. This allows us to obtain simple and precise quantities with a well defined continuum limit. In the case of the φ^4 theory the gradient flow equations can be defined as [10]: $\partial_t\tilde{\varphi}(x,t)=\partial^2\tilde{\varphi}(x,t)$, $\tilde{\varphi}(x,0)=Z_\varphi^{-1/2}\varphi(x)$, where $t\geq 0$ is the flow time, and Z_φ is the wavefunction renormalization. We then consider the dimensionless quantity $\mathscr{E}=t^2\langle E\rangle$, where E is given by the quartic energy density of the field at positive flow time, i.e., $\langle E\rangle=\langle\tilde{\varphi}(x,t)^4\rangle=E_0+E_1g_0+E_2g_0^2+E_3g_0^3+\mathrm{O}(g_0^4)$. In particular, we are interested in studying the continuum limit of $\mathscr{E}$ keeping the box size L, the mass m, and the flow time t, fixed in physical units. To this end, we introduce the dimensionless constants, $z=mL$ and $c=\sqrt{8t}/L$. The continuum limit is then taken by increasing the lattice size L/a and decreasing the lattice mass am, while holding z and c fixed.

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The renormalization of the mass can be fixed by requiring [5],

$$\frac{\chi_2}{\chi_2^*} = \left(1 + \frac{\hat{p}_*^2}{m^2}\right), \qquad p_* = (2\pi/L, 0, 0, 0), \tag{6.1}$$

where $\hat{p}^2 = \sum_\mu \hat{p}_\mu^2$ with $\hat{p}_\mu = 2\sin(p_\mu/2)$, and p_μ are the lattice momenta in a periodic box. χ_2 and χ_2^*, are the connected two-point functions of the field $\varphi(x)$ evaluated at momentum $p = 0$ and p_*, respectively. Once the relation (6.1) is computed as a power series in both δm^2 and g_0, this condition allows us to determine δm^2 as a series in g_0. Finally, the wavefunction renormalization of the bare fields at $t = 0$ can be defined as: $Z_\varphi^{-1} = (\chi_2^{*-1} - \chi_2^{-1})/\hat{p}_*^2$ [5].

7. Results

In Figure 1 we present a check on the consistency of the different methods in the perturbative computation of $\mathscr{E}$. The extrapolations are compared with analytic results where available.

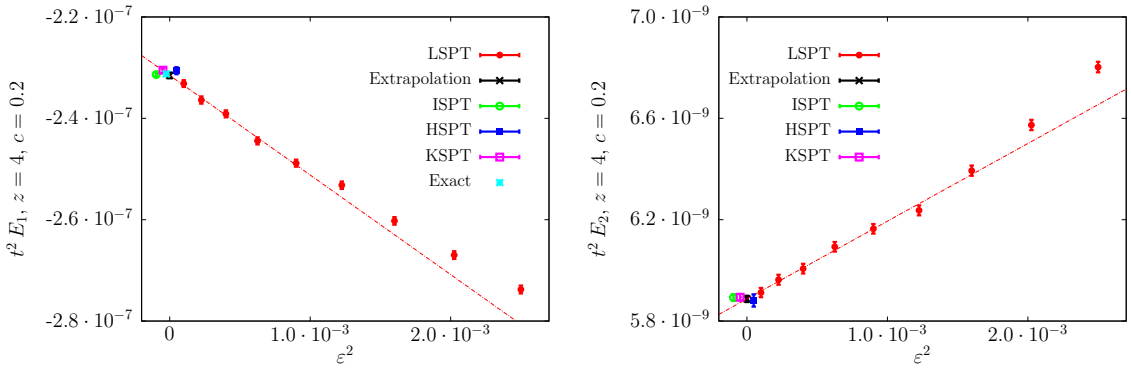

Figure 1: Comparison of different methods in the determination of t^2E_1 and t^2E_2 for $z = 4$, $c = 0.2$, and $L/a = 4$. The analytic result, "Exact", the result of the extrapolation for LSPT, "Extrapolation", as well as the ISPT, KSPT and HSPT results are plotted near $\varepsilon = 0$.

In the figure we show the results for LSPT for different values of the step-size ε, and corresponding extrapolations $\varepsilon \to 0$. The integration of the Langevin equations has been performed using a 2$^{\text{nd}}$ order Runge-Kutta scheme: we therefore expect $O(\varepsilon^2)$ errors in the observables. The results for KSPT and HSPT, have been obtained using a 4$^{\text{th}}$ order symplectic integrator for the MD equations with step-size $\delta t = 0.5$. This is expected to introduce $O(\delta t^4)$ corrections. Given our choices of integrators the results from HSPT, and KSPT show no sign of step-size errors within the statistical accuracy if compared with the analytic results or ISPT. In the case of LSPT, instead, the step-size errors are significant even though the step-sizes considered all satisfy, $\varepsilon^2 < \delta t^4$; nevertheless the results agree with the other methods after extrapolation to $\varepsilon \to 0$.

In Figure 2 we present the continuum scaling of the relative errors $\Delta E_i/E_i$ of the perturbative coefficients of $\mathscr{E}$ as obtained with ISPT, HSPT and LSPT.[2] The relative error is normalized at its value at $L/a = 4$. For the error analysis in HSPT, and LSPT we employed the method described

[2]We note that even though the field and mass are properly renormalized, the expansion coefficients are in terms of the bare coupling g_0. The associated logarithmic divergence, however, is not expected to be relevant for our conclusions.

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in [11]. In the case of LSPT we considered two values of the step-size ε, in order to access the dependence of the results on it. For HSPT, we kept the average trajectory length fixed to $\langle\tau\rangle = 1$, while decreasing the step-size as $(L/a)^{-1/2}$. This was done in order to keep the step-size errors roughly constant as the continuum limit is approached. Finally, for all methods the number of field configurations has been kept fixed as L/a is increased, and always separated by a single step (trajectory) for LSPT (HSPT).

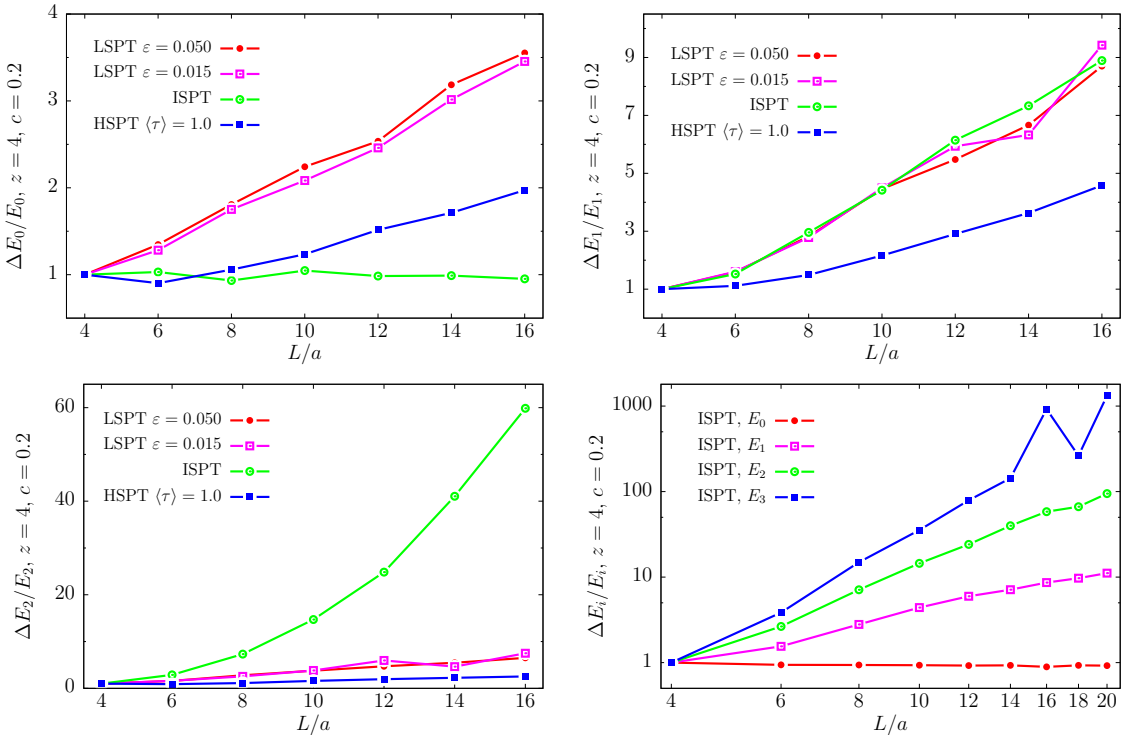

Figure 2: Continuum scaling of the relative errors $\Delta E_i/E_i$ of E_i as computed with ISPT, LSPT and HSPT (see the text for more details). The case with $z = 4$ and $c = 0.2$ is shown.

Observe how the relative errors of $\mathscr{E}$ in LSPT and HSPT grow roughly linearly with L/a. This is compatible with the errors growing due to the increase of autocorrelations as $(L/a)^2$. ISPT, instead, shows a rather different behavior: the relative error of the perturbative coefficients E_i grows as increasing powers of L/a as the perturbative order is increased. This is seen more clearly in the bottom-right panel of Figure 2, where a detail of ISPT is shown. Since in ISPT the field configurations are uncorrelated, this rapid increase in the relative errors of the coefficients must be related to their variance. This behaviour has been elucidated by Lüscher [12], who emphasized the generic presence of power divergences in the variance of perturbative coefficients computed with ISPT; he also shows that such power divergences are excluded if the fields are generated using the Langevin equations. Finally, we investigated how the integrated autocorrelation $A(E_i)$ of the perturbative coefficients E_i scales with L/a in HSPT. In Figure 3 we compare the case $\langle\tau\rangle = 1$ with the case when $\langle\tau\rangle = (am)^{-1}$. For all perturbative orders we considered, the results are consistent with the free field theory expectations [13], namely $A(E_i)$ for $\langle\tau\rangle = 1$ grows like $(L/a)^2$ whereas for $\langle\tau\rangle = (am)^{-1}$ it is constant.

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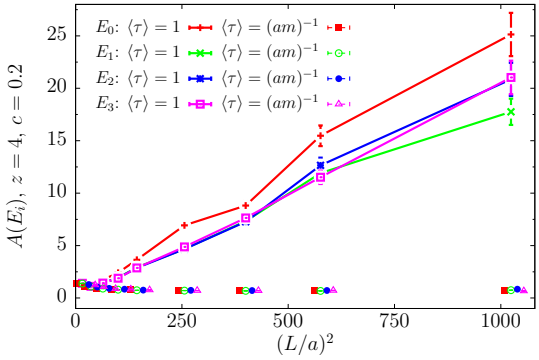

Figure 3: Continuum scaling of the integrated autocorrelations $A(E_i)$ of E_i, $i = 0, \ldots 3$, for the cases $\langle\tau\rangle = 1$ and $\langle\tau\rangle = (am)^{-1}$. The points for $\langle\tau\rangle = (am)^{-1}$ are shifted along the x axis for clarity.

8. Conclusions

From this study we conclude that the variance of ISPT grows very rapidly as we increase the order in g_0. Even though it has many appealing features, this technique does not appear to be competitive in its present form. On the other hand, defining NSPT in terms of different stochastic equations, as the HMD or the Kramers equations, is a simple and profitable idea. Indeed, this allows us to exploit recent algorithmic advances in the context of stochastic perturbation theory. This will be extremely useful for more complicated theories such as QCD.

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