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Towards a determination of c_{SW} using Numerical Stochastic Perturbation Theory (NSPT)

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We outline a strategy to compute the second-loop contribution to the c_{SW} coefficient of the Sheikoleslami-Wohlert-Wilson fermion action by means of NSPT. We also present preliminary results for higher-order integrators for the Langevin evolution within NSPT. At fixed numerical accuracy, these integrators considerably reduce the required computer-time.

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1. Motivation

A problem one has often to face when handling lattice results is taking the continuum limit.

A viable way of reducing the impact of lattice artifacts (by *removing* some of them) is given by the Symanzik improvement programme [1] which, as is well-known, has allowed to remove $\mathscr{O}(a)$ artifacts in unquenched simulations. The irrelevant term to be added to the lattice action was determined by Sheikoleslami and Wohlert [2] and contains the so-called c_{SW} coefficient which can be expanded perturbatively in even powers of the bare coupling g_0.
While the zero- and one-loop coefficients of this expansion have already been computed for different lattice actions [3, 4] (see also references therein), the two-loop contribution is still unknown: within the Wilson formulation of Lattice QCD (LQCD), we address its determination using NSPT, a tool that allows for perturbative calculation in lattice-regularized quantum field theories.

In the second part, we discuss a technical issue of NSPT that is related to the discretization of the Langevin equation that governs the evolution of the system: our target is to obtain high-order integrators, aiming at reducing the computer-time at fixed accuracy.

2. Wilson formulation of LQCD and improvement: some notation

The Wilson action S_W of LQCD can be decomposed into gauge (S_G) and fermionic (S_F) parts with[1],

$$S_G = \beta \sum_{\substack{n,\mu,\nu \\ \mu>\nu}} \left(1 - \frac{Tr}{2N_c}\left[U_{\mu\nu}(n) + U^{\dagger}_{\mu\nu}(n)\right]\right) , \tag{2.1}$$

where $\beta = 2N_c/g_0^2$, N_c is the number of colours, $U_{\mu\nu}(n)$ is the lattice plaquette and,

$$S_F = \sum_{\substack{n,\alpha,b \\ m,\beta,c}} \bar{\psi}_{\alpha b}(n) \mathscr{M}_{n\alpha b,\, m\beta c}[U] \psi_{\beta c}(m) , \tag{2.2}$$

with

$$\begin{aligned} \mathscr{M}[U]_{n\alpha b, m\beta c} = & -\frac{1}{2}\sum_{\mu}\left[(r-\gamma_\mu)_{\alpha\beta}\, U_\mu(n)_{bc}\, \delta_{n+\hat{\mu},m} + (r+\gamma_\mu)_{\alpha\beta}\, U^{\dagger}_\mu(m)_{bc}\, \delta_{n-\hat{\mu},m}\right] + \\ & + (\widehat{M}_0 + 4r)\, \delta_{nm}\, \delta_{\alpha\beta}\, \delta_{bc} . \end{aligned} \tag{2.3}$$

In eq. (2.3), r is the Wilson parameter (which we will set to 1) while $\widehat{M}_0$ is the bare mass.

The Sheikoleslami-Wohlert irrelevant contribution (S_{SW}) to be added to the Wilson action is given by[2],

$$S_{SW} = \frac{i}{4} c_{SW} \sum_{n,\,\mu,\nu} \bar{\psi}(n) \sigma_{\mu\nu} \hat{F}_{\mu\nu}(n) \psi(n) , \tag{2.4}$$

where $\sigma_{\mu\nu} = i/2[\gamma_\mu, \gamma_\nu]$ while $\hat{F}_{\mu\nu}(n)$ reads,

[1] In the equations of this and the subsequent section it is understood that all dimensionful quantities have been rescaled with powers of the lattice spacing a to be dimensionless (some of them carry an extra "hat" to emphasize this).

[2] In the following equations, spin and colour subscripts are suppressed to ease the notation: they can obviously be restored as in eq. (2.3).

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$$\hat{F}_{\mu\nu}(n) = \frac{1}{8}\big(Q_{\mu\nu}(n) - Q_{\nu\mu}(n)\big), \tag{2.5}$$

with $Q_{\mu\nu}(n)$ being the clover term, $Q_{\mu\nu}(n) = U_{\mu,\nu}(n) + U_{-\nu,\mu}(n) + U_{\nu,-\mu}(n) + U_{-\mu,-\nu}(n)$.

As already anticipated, the coefficient c_{SW} appearing in eq. (2.4) can be decomposed as

$$c_{SW} = c_{SW}^{(0)} + c_{SW}^{(1)} g_0^2 + c_{SW}^{(2)} g_0^4 + \mathscr{O}(g_0^6) \ , \tag{2.6}$$

where $c_{SW}^{(2)}$ is the target of our computation.

3. How to measure $c_{SW}^{(2)}$

A suitable observable to determine $c_{SW}^{(2)}$ is given by the pion propagator[3],

$$\begin{aligned} G_{bc}(n-m) &= -\sum_{\alpha,\beta,\delta,\varepsilon} \langle \bar{\psi}_{\alpha b}(n)(\gamma_5)_{\alpha\beta}\psi_{\beta b}(n)\bar{\psi}_{\delta c}(m)(\gamma_5)_{\delta\varepsilon}\psi_{\varepsilon c}(m)\rangle = \\ &= \sum_{\alpha,\beta,\delta,\varepsilon} \langle (\gamma_5)_{\alpha\beta}\Big[\tilde{M}^{-1}\Big]_{n\beta b,\, m\delta c}(\gamma_5)_{\delta\varepsilon}\Big[\tilde{M}^{-1}\Big]_{m\varepsilon c,\, n\alpha b}\rangle_U = \\ &= \sum_{\alpha,\varepsilon} \langle \Big[\tilde{M}^{-1}\Big]^*_{m\varepsilon c,\, n\alpha b}\Big[\tilde{M}^{-1}\Big]_{m\varepsilon c,\, n\alpha b}\rangle_U = \sum_{\alpha,\varepsilon}\langle \left|\Big[\tilde{M}^{-1}\Big]_{m\varepsilon c,\, n\alpha b}\right|^2\rangle_U, \end{aligned} \tag{3.1}$$

where $\tilde{M}$ is the fermionic operator obtained by adding together eqs. (2.2) and (2.4): for details about its inversion, see [5]. After switching to momentum space and defining the dimensionless quantities $\hat{p}_\mu = p_\mu a$ and $\hat{p}^2 = \sum_\mu \hat{p}_\mu^2$ (being the p_μ's the lattice momentum components), one can invert the propagator to obtain the $\hat{\Gamma}$-function which can be decomposed as,

$$\hat{\Gamma}(\hat{p}, \hat{m}_{cr}, g_0) = \hat{p}^2 + \widehat{M}_0^2 + \widehat{M}_W^2(\hat{p}) - \hat{\Sigma}(\hat{p}, \hat{m}_{cr}, g_0) \ , \tag{3.2}$$

where $\widehat{M}_W(\hat{p})$ is the irrelevant Wilson mass, $\widehat{M}_0$ the (perturbative) pion rest mass and $\hat{\Sigma}(\hat{p}, \hat{m}_{cr}, g_0)$ the self-energy with $\hat{m}_{cr}$ the critical mass defined as $\hat{m}_{cr} = \hat{\Sigma}(0, \hat{m}_{cr}, g_0)$. Since we want to develop a mass-independent scheme, we will both set $\widehat{M}_0$ equal to zero and subtract the proper mass counterterms to keep fermions massless.

Given that we are eventually interested in a perturbative approach, we can expand $\hat{\Sigma}(\hat{p}, \hat{m}_{cr}, g_0)$ as a series in g_0^2, i.e. $\hat{\Sigma}(\hat{p}, \hat{m}_{cr}, g_0) = \sum_k \hat{\Sigma}^{(k)}(\hat{p}, \hat{m}_{cr}) g_0^{2k}$, and decompose a generic coefficient $\hat{\Sigma}^{(k)}(\hat{p}, \hat{m}_{cr})$ by means of *hypercubic invariants* as,

$$\hat{\Sigma}^{(k)}(\hat{p}, \hat{m}_{cr}) = \alpha_1^{(k)}(\hat{m}_{cr}) + \alpha_2^{(k)}(\hat{m}_{cr}) \sum_\rho \hat{p}_\rho^2 + \alpha_3^{(k)}(\hat{m}_{cr}) \sum_\rho \hat{p}_\rho^4 + \dots \ . \tag{3.3}$$

A possible approach to determine $c_{SW}^{(2)}$ would consist of expanding the pion and quark self energies[4] in a combined way: one could take $c_{SW}^{(0)} = 1$ to obtain κ_c to $\mathscr{O}(\beta^{-1})$, then take this value to tune $c_{SW}^{(1)}$ to make the pion mass vanish; next, one revisits the quark propagator to determine κ_c to $\mathscr{O}(\beta^{-2})$ and so on till $c_{SW}^{(2)}$ is determined[5].

[3] The subscript "U" means that the corresponding average has to be performed on gauge configurations only.

[4] Formulae similar to eqs. (3.2)–(3.3) hold also for the quark propagator though the Dirac structure is more involved.

[5] It is clear that, requiring the pion to be massless, also implies setting $\widehat{M}_0^2$ equal to zero.

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An alternative strategy could be the following: recall that S_{SW} was introduced to remove $\mathcal{O}(a)$ artifacts and the pion propagator contains the product of two quark propagators. One should be able to establish a correspondance between terms proportional to a in the operator $\tilde{M}^{-1}$ and the ones proportional to a^2 in the $\hat{\Gamma}$-function, namely $\alpha_3^{(k)}$. If one now tunes $c_{SW}^{(0)}$ and $c_{SW}^{(1)}$ to their known values and observes that, correspondingly, $\alpha_3^{(1)}$ and $\alpha_3^{(2)}$ vanish, one can fix $c_{SW}^{(2)}$ by requiring $\alpha_3^{(3)}$ to be zero. This approach is maybe less rigorous but nonetheless should be worth studying.

4. Numerical setup

The method of our choice is NSPT. It is related to *Stochastic Quantization* [6] which consists of introducing an extra coordinate, a stochastic time t, together with an evolution equation of the Langevin type,

$$\frac{\partial\phi(x,t)}{\partial t} = -\frac{\partial S[\phi]}{\partial\phi} + \eta(x,t) \ , \tag{4.1}$$

where in this example $\phi(x,t)$ is a scalar field while $\eta(x,t)$ is a Gaussian noise.
Starting from this, the usual Feynman-Gibbs integration can be recovered by noise-averaging as

$$Z^{-1}\int [D\phi]O[\phi(x)]e^{-S[\phi(x)]} = \lim_{t\to\infty}\frac{1}{t}\int_0^t \mathrm{d}t' \left\langle O[\phi_\eta(x,t')]\right\rangle_\eta \ . \tag{4.2}$$

For $SU(3)$ lattice variables the Langevin equation has to be modified into [5],

$$\partial_t U_\mu(n,t) = -iT^A\Big(\nabla_{n,\,\mu,\,A}S[U] + \eta_\mu^A(n,t)\Big)U_\mu(n,t) \ , \tag{4.3}$$

in order to obtain an evolution of the variables within the group: here $T^A = \lambda^A/2$ are Gell-Mann matrices while $\eta_\mu^A(n,t)$ are again Gaussian noise components.

The missing ingredient, i.e. Perturbation Theory, is introduced by expanding the U's as[6],

$$U_\mu(x,t) \longrightarrow \sum_k \beta^{-\frac{k}{2}} U_\mu^{(k)}(x,t) \ , \tag{4.4}$$

When plugging this into the Langevin equation, this results in a system of coupled differential equations that can be solved numerically via a discretization of the stochastic time $t = N\tau$, where τ is a time step.

In practice, the system is evolved for different values of τ, then we average over each thermalized signal to realize the limit $t\to\infty$ of eq. (4.2). Finally we extrapolate in τ to the $\tau = 0$ limit of the desired observable: this extrapolation is needed since *the correct Boltzmann equilibrium distribution is recovered only for continuous t*.

5. High-order integrators for NSPT

The c_{SW}-simulations are an ongoing project such that the numerical results presented here refer to improvements of the NSPT algorithm.

[6]The expansion in the computer code is thought on $\beta^{-1/2}$ rather than g_0: converting the corresponding coefficients is obviously straightforward.

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As mentioned above, one has to perform simulations with different values of τ to extrapolate towards the limit $\tau \to 0$ and this increases the required computer-time. Since the smaller τ is, the more iterations N are needed, a possible way to save computer-time might consist of employing larger values of τ; however, this would compromise the accuracy of the subsequent τ-extrapolation. The solution to this drawback is well-known and is represented by *high-order integrators* for the Langevin equation: these indeed increase the power of the leading τ-dependence thus allowing to safely recover the $\tau \to 0$ limit even at large values of the time step.

The easiest way of determining high-order integrators is probably by generalizing the usual Runge-Kutta schemes for the scalar case: there, given a scalar variable $y(\tau)$, its derivative $y' = f(\tau,y)$ and an initial value $y(\tau_0) \equiv y_0$, the m-th order integrator reads:

$$y_{n+1} = y_n + \tau \sum_{l=1}^{m} b_l k_l \qquad \left(k_l = f\left(\tau_n + c_l \tau, y_n + \tau \sum_{r=1}^{l-1} a_{l,r} k_r\right) \;;\; k_1 = f(\tau_n, y_n)\right) , \tag{5.1}$$

The generalization to non-Abelian variables appears straightforward:

$$y_{n+1} = y_n + \tau \sum_{l=1}^{m} b_l k_l \longrightarrow U_\mu(x,\tau_{n+1}) = \exp\left[-i\tau \sum_{l=1}^{m} b_l \Big(\eta_\mu(x,\tau_n) + \tilde{k}_l \Big)\right] U_\mu(x,\tau_n) , \tag{5.2}$$

$$k_l = f\left(\tau_n + c_l\tau \, , \, y_n + \tau \sum_{r=1}^{l-1} a_{l,r} k_r\right) \longrightarrow \tilde{k}_l = \sum_A T^A \nabla_{x,\mu,A} S[\, \widetilde{U}^{(l)}] \, , \tag{5.3}$$

where $S[\widetilde{U}^{(l)}]$ is the expression of the action where all variables have been replaced as

$$U_\mu(x,\tau_n) \longrightarrow \exp\left[-i\tau \sum_{r=1}^{l-1} a_{l,r} \left(\eta_\mu(x,\tau_n) + \tilde{k}_r \right)\right] U_\mu(x,\tau_n) \, , \tag{5.4}$$

where it is understood that $\tilde{k}_1 = \sum_A T^A \nabla_{x,\mu,A} S[U(\tau_n)]$.
As is manifest, the number of operations per update increases with the order of the integrator: one will eventually be able to employ larger time steps in the simulations, thus reducing the number of iterations, but at the price of more costly iterations. Our study seems to indicate that overall savings of up to a factor of two can still be achieved.

Now everything boils down at getting the coefficients $a_{l,r}, b_l, c_l$ in eq. (5.1) but they can easily be found in the literature.

At present, the highest integrator available for the NSPT Langevin equation is second-order [7] and reads,

$$U_\mu(x,\tau_{n+1}) \; = \; exp\left[-i\left(1 + \frac{\tau C_A}{6\beta}\right)\left(\frac{1}{2}\tau\tilde{k}_1 + \frac{1}{2}\tau\tilde{k}_2\right) - i\sqrt{\tau}\eta_\mu(x,\tau_n)\right] U_\mu(x,\tau_n) \, , \tag{5.5}$$

$$\tilde{k}_1 \; = \; \sum_A T^A \nabla_{x,\mu,A} S[U(\tau_n)] \, , \tag{5.6}$$

$$\tilde{k}_2 \; = \; \sum_A T^A \nabla_{x,\mu,A} S[\widetilde{U}^{(2)}] \, , \tag{5.7}$$

$$\widetilde{U}^{(2)}_\mu(x,.) \; = \; exp\Big[-i\tau\tilde{k}_1 - i\sqrt{\tau}\eta_\mu(x,\tau_n)\Big] U_\mu(x,\tau_n) \, , \tag{5.8}$$

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where C_A is the Casimir invariant of the Lie group's adjoint representation: note that the noise employed in eqs. (5.5) and (5.8) is the same. The second term in the first square brackets in eq. (5.5) — not appearing in Runge-Kutta literature — comes from the non-commutativity of group derivatives introduced in eq. (4.3). Apart from a rescaling[7] of τ with β [5], the integrator can be determined by calculating the equilibrium distribution of the corresponding discretized *Fokker-Planck equation*.

At present, analytical calculations are undertaken in order to compute the corresponding non-Abelian shifts for both the third- and the fourth-order integrator.

6. Preliminary results

As can be seen from eq. (5.5), the above-mentioned non-Abelian shift only affects loops higher than the first and thus we are already in the position of comparing one-loop results obtained with different integrators: the variable we choose is the plaquette at a lattice extent $L = 4$.
Figure 1 shows how the slope in τ changes with the integrator as expected while, in Table 1, we collect our numerical results: as desired, the accuracy remains rather good even when employing larger τ values in the simulations.

Order of integrator	Employed time steps	1-loop plaquette
1	10, 15, 20	1.9930(7)
2	50, 60, 70	1.9922(6)
3	90, 100, 110	1.9918(10)
4	110, 122, 130	1.9914(10)

Table 1: Comparison between 1-loop results for different integrators at L=4. the diagrammatic $L = 4$ value reads 1.9921875....

The second-order integrator should already be working to any perturbative order so that, as a second test, we can check whether higher loops are under control too when increasing the time steps in the simulations: this is done in Table 2 where benchmark plaquette results at $L = 4$ are provided by the first-order integrator that has been in use since long.

Order of integrator	1st loop	2nd loop	3rd loop	4th loop
1	1.9930(7)	1.2027(18)	2.8781(67)	8.994(30)
2	1.9922(6)	1.2002(17)	2.8778(62)	8.990(28)

Table 2: $\tau \to 0$ results from 1st and 2nd order integrators at $L = 4$: the 1- and 2-loop diagrammatic values read 1.9921875... and 1.2037037.... The time steps employed can be found in Table 1.

In Figure 2 we compare the $\tau \to 0$ results from the second order integrator to the corresponding diagrammatic results for different L. At $L = 2$ there is some disagreement which might be due to different ways of treating zero modes. The ratios of diagrammatic finite over infinite volume results

[7] The β prefactor within eq. (2.1) needs to be compensated for and, consequently, the rescaling $\tau \mapsto \tau/\beta$ is required in *every* integration scheme, including Euler's most trivial one.

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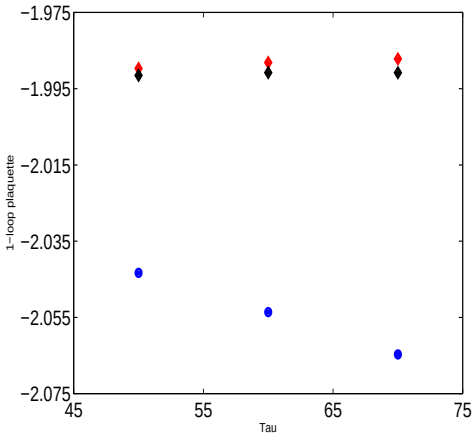

Figure 1: 1-loop plaquette vs. τ at L=4: data come from first-, second- and third-order integrator (blue, red and black points respectively).

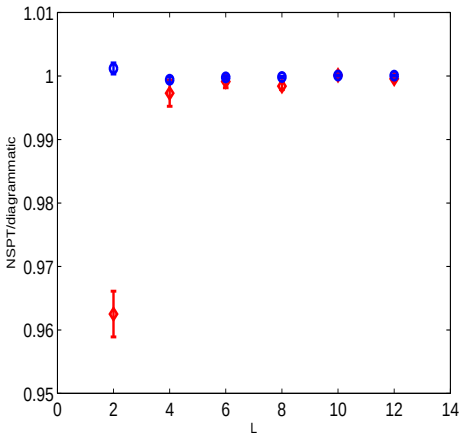

Figure 2: Ratio NSPT results/diagrammatic values vs. L for the 1- and 2-loop plaquette (blue dots and red diamonds respectively).

read 0.907 (0.907) for $L = 2$ and 0.994 (0.986) for $L = 4$ at 1-loop (2-loop) level, respectively: finite volume effects are much bigger than this disagreement between diagrammatic results (neglecting zero modes) and NSPT (subtracting zero modes). The infinite volume limit remains unaffected.

7. Conclusions

The computation of $c_{SW}^{(2)}$ is at an early stage: at present, we are trying to single out the most reliable approach.

As for higher-order integrators for the Langevin equation, first results seem to confirm good gains in computer-time, without any loss in numerical accuracy.

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