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NSPT calculations in the Schrödinger Functional formalism

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Within the framework of the Schrödinger Functional (SF), we outline how to combine Numerical Stochastic Perturbation Theory (NSPT) and PCAC relations to determine the two-loop contributions to the improvement coefficients c_A and c_{SW} for Sheikholeslami-Wohlert-Wilson fermions.

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1. Introduction

As it is well-known, in the improvement approach à la Symanzik [1] the lattice QCD action has to be provided with an extra irrelevant contribution, the so-called *Sheikholeslami-Wohlert term* [2]. In Perturbation Theory (PT), it features a scalar coefficient c_{SW} which can be Taylor-expanded in powers of the bare coupling g_0 as

$$c_{SW} = c_{SW}^{(0)} + c_{SW}^{(1)} g_0^2 + c_{SW}^{(2)} g_0^4 + \mathscr{O}(g_0^6) \ . \tag{1.1}$$

The zero- and one-loop coefficients have already been determined for different lattice actions [3][4] while $c_{SW}^{(2)}$ is still unknown: the final aim of this project is precisely to estimate it by combining the *Schrödinger Functional formalism* (SF) and the *PCAC relations* in the same spirit as [5] and [6] where $c_{SW}^{(0)}$ and $c_{SW}^{(1)}$ were successfully recovered.

The main difference with these two latter seminal papers lies in the fact that observables are evaluated perturbatively without following a diagrammatic approach but rather by means of *Numerical Stochastic Perturbation Theory* (NSPT), a computer algorithm characterized by a Langevin-like evolution of the system.

2. Theoretical aspects - part I (basics)

The lattice formulation of QCD we adopt is that of Wilson: a concrete expression of the well-known contributions to the action - namely the gauge (S_G), fermionic (S_F) and Sheikholeslami-Wohlert (S_{SW}) term - can be found in [5] whose notations and conventions inspire nearly all the formulae appearing in this and the next section [1].

A suitable observable to study in order to evaluate $c_{SW}^{(2)}$ is provided by the quark mass m_q which can be conveniently computed by means of the lattice PCAC relation reading, [2]

$$\frac{1}{2}(\partial_0^R + \partial_0^L)\langle A_0^b(n)\mathbb{O}\rangle = 2m_q\langle P^b(n)\mathbb{O}\rangle \ , \tag{2.1}$$

where $\mathbb{O}$ is any product of fields located at nonzero distance from n, ∂_0^R (∂_0^L) is the lattice right (left) derivative in the time direction and

$$A_0^b(n) = \sum_{f,g}^{N_f} \overline{\psi}^f(n)\gamma_\mu\gamma_5 \frac{1}{2}\tau_{fg}^b \psi^g(n) \ , \qquad P^b(n) = \sum_{f,g}^{N_f} \overline{\psi}^f(n)\gamma_5 \frac{1}{2}\tau_{fg}^b \psi^g(n) \ , \tag{2.2}$$

where τ^b is a matrix acting on flavour degrees of freedom [3].

In order to fix $c_{SW}^{(2)}$, one requires m_q to be independent of contributions of order a: however, to achieve full improvement Eq.(2.1) has to be modified to,

$$\frac{1}{2}(\partial_0^R + \partial_0^L)\langle A_0^b(n)\mathbb{O}\rangle + c_A \partial_0^L \partial_0^R \langle P^b(n)\mathbb{O}\rangle \ = \ 2m_q\langle P^b(n)\mathbb{O}\rangle \ , \tag{2.3}$$

[1] More generally, we stick to the setup outlined in sections 2, 4 and 6 of [5].
[2] From now on, the time direction will be assigned the subscript 0.
[3] Spin and colour subscripts will be usually left implicit in order to ease the notation.

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where c_a is a second improvement coefficient which, just like c_{SW}, can also be decomposed as $c_A = c_A^{(0)} + c_A^{(1)} g_0^2 + c_A^{(2)} g_0^4 + \mathscr{O}(g_0^6)$. Once again, the first unknown contribution is at two-loop level: see [5] and [6] for the determination of $c_A^{(0)}$ and $c_A^{(1)}$.

The second main theoretical ingredient of the present strategy is given by the Schrödinger Functional: assuming the time coordinate ranges from 0 to T and labelling the space coordinates as $\vec{n}$, it consists of replacing the usual periodic boundaries by Dirichlet conditions along the time direction, namely,

$$U_k(n)|_{n_0=0} \to W_k(\vec{n}) \;, \qquad U_k(n)|_{n_0=T} \to W'_k(\vec{n}) \quad (k=1,2,3) \;, \tag{2.4}$$

for the gauge degrees of freedom[4] and ($P_\pm = (\mathbb{I} \pm \gamma_0)/2$ with $\mathbb{I}$ being the identity matrix)

$$\psi^f(n)\big|_{n_0=0} \to \rho^f(\vec{n}) = P_+ \psi^f(n)\big|_{n_0=0} \;, \qquad \psi^f(n)\big|_{n_0=T} \to \rho'^f(\vec{n}) = P_+ \psi^f(n)\big|_{n_0=T} \;, \tag{2.5}$$

$$\overline{\psi}^f(n)\big|_{n_0=0} \to \overline{\rho}^f(\vec{n}) = P_+ \overline{\psi}^f(n)\big|_{n_0=0} \;, \qquad \overline{\psi}^f(n)\big|_{n_0=T} \to \overline{\rho}'^f(\vec{n}) = P_+ \overline{\psi}^f(n)\big|_{n_0=T} \;, \tag{2.6}$$

for fermions: boundary fields W, W', ρ, $\overline{\rho}$, ρ' and $\overline{\rho}'$ will be defined later on.

Due to the Schrödinger Functional formalism, the three contributions to the lattice QCD action get modified as follows:

- the gauge part S_G becomes

$$S_G = \beta \sum_{\substack{n,\mu,\nu \\ \mu>\nu}} \omega_{\mu\nu}(n) \left(1 - \frac{Tr}{2N_c}\left[U_{\mu\nu}(n) + U^\dagger_{\mu\nu}(n)\right]\right) \;, \tag{2.7}$$

  where the weight $\omega_{\mu\nu}(n)$ for the lattice plaquette $U_{\mu\nu}(n)$ is 1 everywhere except for the spatial plaquette at $n_0 = 0$ and $n_0 = T$ whose $\omega_{\mu\nu}(n)$ reads $\frac{1}{2}$;

- the fermionic part S_F remains in principle unchanged; anyway, in order to have one more parameter to play with, an additional phase $e^{i\theta_\mu/L_\mu}$ is introduced in the definition of the lattice covariant derivatives within the Wilson-Dirac operator: in practice, gauge fields $U_\mu(n)$ appearing in S_F are replaced by,

$$U_\mu(n) \to e^{i\theta_\mu/L_\mu} U_\mu(n) \;, \tag{2.8}$$

  with $\theta_0 = 0$ and $-\pi < \theta_k \leq \pi$ for $k = 1,2,3$;

- the clover term is set to 0 for all those lattice points with $n_0 = 0$ or $n_0 = T$.

[4] Gauge fields along the time direction, defined for $0 \leq n_0 < T$, have no constraints on them. It turns out that W and W' can sloppily be written as $W = \mathscr{P}e^{\int C}$ and $W = \mathscr{P}e^{\int C'}$ - see section 6 of [5] for notations and a more careful and detailed treatment of this topic - where C and C' play a similar role as the background field in classical physics: in what follows we will refer to the case $C = C' = 0$ as the *trivial background*.

3. Theoretical aspects - part II (details)

Before outlining the procedure that should lead to an estimate of $c_{SW}^{(2)}$, let us give a precise shape to the observable $\mathbb{O}$ appearing in Eq.(2.3): a convenient choice reads,

$$\mathbb{O} = a^6 \sum_{f,g}^{N_f} \sum_{\vec{m},\vec{m}'} \overline{\varsigma}^f(\vec{m}) \gamma_5 \frac{1}{2} \tau^b_{fg} \varsigma^g(\vec{m}') \; , \tag{3.1}$$

where

$$\varsigma^f(\vec{m}) = \frac{\delta}{\delta \overline{\rho}^f(\vec{m})} \; , \qquad \overline{\varsigma}^f(\vec{m}) = -\frac{\delta}{\delta \rho^f(\vec{m})} \; . \tag{3.2}$$

After first plugging Eq.(3.1) into Eq.(2.3), then letting the derivatives with respect to ρ and $\overline{\rho}$ act on the Boltzmann factor and finally setting all the fermionic boundary fields to zero, some algebra allows one to write

$$m_q = \frac{\frac{1}{2}\left[\frac{1}{2}(\partial_0^R + \partial_0^L) f_A + c_A \partial_0^L \partial_0^R f_P\right]}{f_P} \; , \tag{3.3}$$

with[5]

$$f_A = \frac{1}{12} \sum_{\vec{m},\vec{m}'} \langle H^{lf}_{[(\vec{m}+\hat{0})\,\omega c\,,\, n \varepsilon e]} \, (\gamma_0)_{\varepsilon\beta} \; \tau^b_{fg} \, (P_-)_{\omega\sigma} \; J^{gh}_{[(\vec{m}'+\hat{0})\,\sigma c\,,\, n \beta e]} \; \tau^b_{hl} \rangle_G \; , \tag{3.4}$$

$$f_P = \frac{1}{12} \sum_{\vec{m},\vec{m}'} \langle H^{lf}_{[(\vec{m}+\hat{0})\,\omega c\,,\, n \varepsilon e]} \; \tau^b_{fg} \, (P_-)_{\omega\sigma} \; J^{gh}_{[(\vec{m}'+\hat{0})\,\sigma c\,,\, n \varepsilon e]} \; \tau^b_{hl} \rangle_G \; , \tag{3.5}$$

with

$$H^{lf}_{[(\vec{m}+\hat{0})\,\omega c\,,\, n \varepsilon e]} = \Big[U_0(\vec{m})\Big]_{cb} \left(\widetilde{M}^{-1}\right)^{lf}_{[(\vec{m}+\hat{0})\,\omega b\,,\, n \varepsilon e]} \; , \tag{3.6}$$

$$J^{gh}_{[(\vec{m}'+\hat{0})\,\sigma c\,,\, n \beta e]} = \Big[U_0(\vec{m}')\Big]^*_{cd} \left(\widetilde{M}^{-1^*}\right)^{gh}_{[(\vec{m}'+\hat{0})\,\sigma d\,,\, n \beta e]} \; , \tag{3.7}$$

where $\widetilde{M}$ is the overall fermionic opearator in the lattice action.

f_A, f_P and m_q depend on the lattice spacing a, the lattice extents L_μ, the bare coupling g_0, the gauge fields W and W', the angles θ_k (from now on, we will set the latter equal to a common value θ) and the improvement coefficients: recalling that the approach is perturbative, we can write[6],

$$m_q(L,\theta,x_0,g_0,a) = m_q^{(0)}(L,\theta,x_0,a) + m_q^{(2)}(L,\theta,x_0,a) g_0^2 + m_q^{(4)}(L,\theta,x_0,a) g_0^4 + \mathscr{O}(g_0^6) \; , \tag{3.8}$$

[5] The subscript “G" stands for the mean over gauge degrees of freedom. Here and in Eqs.(3.6)-(3.7) repeated indices are summed over. Moreover, from now on we tacitly assume that all quantities are rescaled with a to be dimensionless.

[6] We make the dependence on W, W', c_{SW} and c_A implicit not to overwhelm the notation; at the same time, we drop the subscript on the lattice extents for a reason that will become clear soon.

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and in turn, thanks to dimensional analysis

$$m_q^{(k)}(L,\theta,x_0,a) = d_L(c_{SW}^{(i\le k)},c_A^{(i\le k)})\frac{a}{L} + d_{x_0}(c_{SW}^{(i\le k)},c_A^{(i\le k)})\frac{a}{x_0} + d_\theta(c_{SW}^{(i\le k)},c_A^{(i\le k)})\frac{a\theta}{L} + \mathscr{O}(a^2)\ . \quad (3.9)$$

This formula can actually be simplified by setting the L_k's to the same value L, putting $L_0 = 2L$ and choosing $n_0 = L$: thus, the corrections in a to $m_q^{(k)}$ will be grouped together into a single one proportional to a/L. Since the aim of improvement is to get rid of lattice artifacts of order a, it is reasonable to estimate $c_{SW}^{(2)}$ by requiring the only coefficient $d(c_{SW}^{(i\le k)},c_A^{(i\le k)})$ left in the formula above - after its reduction - to vanish. This can be achieved by the following steps: 1) fix $c_{SW}^{(2)}$ and $c_A^{(2)}$ arbitrarily after setting $c_{SW}^{(0)}$, $c_{SW}^{(1)}$, $c_A^{(0)}$ and $c_A^{(1)}$ to their known values; 2) perform simulations for different lattice extents keeping θ, W and W' constant; 3) fit the coefficient $d(c_{SW}^{(2)},c_A^{(2)})$; 4) repeat the previous steps for different choices of $c_{SW}^{(2)}$ and $c_A^{(2)}$; 5) collect the various estimates of $d(c_{SW}^{(2)},c_A^{(2)})$ and interpolate the values of $c_{SW}^{(2)}$ and $c_A^{(2)}$ for which $d(c_{SW}^{(2)},c_A^{(2)})$ vanishes.

Before ending this section, some remarks are in order.

The first term on the r.h.s.of Eq.(3.8) should normally correspond to the bare mass $\widehat{M}_0$ appearing in S_F; however, in the present setup, *this is the case only if* $\theta = 0$: we chose to set $\widehat{M}_0 = 0$ but to work with non-vanishing θ to avoid any infrared divergence.

Second, in Eq.(3.9) it is understood that mass counterterms - depending on c_{SW} [7] - are subtracted. Otherwise $m_q^{(k)}$ would not be 0 in the large L limit: this subtraction prevents extra improvement coefficients to appear (see section 3 in [5]) but, in practice, this should really matter only when working with renormalized quantities (while we deal with their bare counterparts).

Finally, it is possible to disentangle the effects of $c_{SW}^{(2)}$ and $c_A^{(2)}$ by means of W and W': in particular it turns out that, if the *trivial background* (see footnote 4) is set, only $c_A^{(2)}$ has an effect at two-loop level. We start with this choice of the boundary gauge fields to fix this coefficient, afterwards W and W' will be changed to determine $c_{SW}^{(2)}$ thanks also to the by-then-known estimate of $c_A^{(2)}$.

4. Numerical aspects

Two more issues have still to be addressed about the present strategy, namely how configurations are generated and how the Wilson-Dirac operator is inverted to compute f_A and f_P eventually: to answer both, we must introduce some basics of NSPT [7].

Its core is given by the Langevin evolution equation that, for lattice gauge variables [8], reads

$$\frac{\partial}{\partial t}U_\mu(n,t) = -i\sum_A T^A\left[\nabla_{n,\mu,A}S[U] + \eta_\mu^A(n,t)\right]U_\mu(n,t)\ , \quad (4.1)$$

where t is an extra degree of freedom (which can be thought as a *stochastic time*), S is the part of the lattice action depending on the U's, η is a Gaussian noise while ∇ stands for the group derivative

[7] See [8] and references therein for more details on this section in general.

[8] As usual, fermion fields are integrated out so that only gauge degrees of freedom have to be eventually treated.

defined as (index "A" is summed over),

$$\mathscr{F}\left[e^{i\,\alpha^A T^A} U_\mu(n), U'\right] = \mathscr{F}\left[U_\mu(n), U'\right] + \alpha^A \nabla_{n,\mu,A}\, \mathscr{F}[U_\mu(n), U'] + \dots\ , \tag{4.2}$$

where T^A are the generators of the algebra and $\mathscr{F}$ is a generic scalar function of both the variable $U_\mu(n)$ and some more labelled U' for short.

Given this setup, it can be shown that

$$Z^{-1}\int [DU] O[U] e^{-S[U]} = \lim_{t\to\infty} \frac{1}{t}\int_0^t \mathrm{d}t' \left\langle O[U_\eta(t')]\right\rangle_\eta\ , \tag{4.3}$$

where Z is the partition function and $O[U]$ a generic observable depending on the gauge fields.

Perturbation theory enters into play by *formally* expanding each gauge degree of freedom in powers of β_0^{-1} - defined as $\beta_0 = 2N_c/g_0^2$ being N_c the number of colours - up to a given order s as

$$U_\mu(n,t) = \mathbb{I} + \sum_{k=1}^{s} \beta_0^{-\frac{k}{2}} U_\mu^{(k)}(n,t)\ , \tag{4.4}$$

and then plugging this Taylor series [9] into Eq.(4.1): this results in a consistent *hierarchical system of differential equations* which can be numerically integrated by discretizing the stochastic time as $t = n\tau$ with n integer. In practice, the system starts from an arbitrary configuration and evolves by means of the solution of the discretized counterpart of Eq.(4.1): the desired observable is then obtained by averaging its measurements on its plateau - recall the limit in t in Eq.(4.3) [10].

As for the inverse of the fermionic operator, the entries needed to get f_A and f_P can be computed by means of the following perturbative formulae

$$\begin{aligned}
\widetilde{M}^{-1^{(0)}} &= \widetilde{M}^{(0)^{-1}}\ ,\\
\widetilde{M}^{-1^{(1)}} &= -\widetilde{M}^{(0)^{-1}}\widetilde{M}^{(1)}\widetilde{M}^{(0)^{-1}}\ ,\\
\widetilde{M}^{-1^{(2)}} &= -\widetilde{M}^{(0)^{-1}}\widetilde{M}^{(2)}\widetilde{M}^{(0)^{-1}} + \\
&\quad -\widetilde{M}^{(0)^{-1}}\widetilde{M}^{(1)}\widetilde{M}^{-1^{(1)}}\ ,\\
&\dots
\end{aligned}$$

where only the zeroth order of $\widetilde{M}$ has to be truly inverted: its expression for trivial W and W' can be found in section 3.1 of [6].

5. Preliminary results

To test the correctness of the overall setup, we computed the one-loop contribution to m_q without any counterterm subtraction for different choices of θ and $c_{SW}^{(0)}$ [11] and compared the results

[9] Strictly speaking, Eq.(4.3) is valid only if the boundary gauge fields are set to the identity as in this first part of the study; once that a non-trivial *background field* is introduced, the expansion would read $U_\mu(n,t) = exp[(C_k' - C_k)/T]\cdot$ $\cdot\,[\mathbb{I} + \sum_k \beta^{-\frac{k}{2}} U_\mu^{(k)}(n,t)]$ - consult section 6.2 in [5] for the meaning of the first term in this product.

[10] This relation is true only for continuous t so that simulations with different τ values have to be performed in order to extrapolate to $\tau \to 0$ afterwards.

[11] This is indeed the only c_{SW} contribution that enters into play at this order with trivial W and W'.

with the analytical values in Table 1.

θ	$c_{SW}^{(0)} = 0.0$	$c_{SW}^{(0)} = 1.0$	$c_{SW}^{(0)} = 1.5$
1.40	2.67621(4)	1.67151(2)	0.94999(1)
1.00	2.63837(3)	1.64808(1)	0.93229(1)
0.45	2.60727(3)	1.62694(1)	0.91948(1)
0.00	2.60571	1.62045	0.91067

Table 1: Numerical results for $m_q^{(1)}$ on a $10^3 * 21$ lattice with $c_A^{(0)} = c_A^{(1)} = 0$: the last line contains the infinite-volume results obtained from [7].

It is reassuring that, when varying $c_{SW}^{(0)}$, outputs change accordingly: the still-existing gap is explained by recalling that finite-size effects are still present and that the analytical results correspond to $m_q^{(0)} = 0$ while in our simulations $m_q^{(0)} \neq 0$ due to the non-vanishing values of θ ($m_q^{(0)}$ approaches with decreasing θ [12] the analytical infinite-volume values computed with $\theta = 0.0$).

6. Conclusions and acknowledgements

According to the first, preliminary results, the outlined approach seems to be feasible: however, since different extrapolations (in τ and L) and interpolations (in $c_A^{(2)}$ and $c_{SW}^{(2)}$ when dealing with non-trivial W and W') are needed, extra care will have to be paid not to spoil accuracy.

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[12] An analytical expression for $m_q^{(0)}$ can be found in section 3 of [6].