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.
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

$$c_{SW} = c_{SW}^{(0)} + c_{SW}^{(1)} g_0^2 + c_{SW}^{(2)} g_0^4 + \mathcal{O}(g_0^6) .$$  (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,\(^2\)

$$\frac{1}{2} (\partial_R^0 + \partial_L^0) \langle A_b^0(n) \rangle = 2m_q \langle P^b(n) \rangle ,$$  (2.1)

where $\mathcal{O}$ is any product of fields located at nonzero distance from $n$, $\partial_R^0$ ($\partial_L^0$) is the lattice right (left) derivative in the time direction and

$$A_b^0(n) = \sum_{f,g} N_f \bar{\psi}^f(n) \gamma_\mu \gamma_5 \frac{1}{2} \tau^b_{fg} \psi^g(n) , \quad P^b(n) = \sum_{f,g} N_f \bar{\psi}^f(n) \gamma_\mu \gamma_5 \frac{1}{2} \tau^b_{fg} \psi^g(n) ,$$  (2.2)

where $\tau^b$ 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,

$$\frac{1}{2} (\partial_R^0 + \partial_L^0) \langle A_b^0(n) \rangle + c_A \partial_R^0 \partial_L^0 \langle P^b(n) \rangle = 2m_q \langle P^b(n) \rangle ,$$  (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.
where $c_A$ is a second improvement coefficient which, just like $c_{SW}$, can also be decomposed as $c_A = c_A^{(0)} + c_A^{(1)} g_0^2 + c_A^{(2)} g_0^4 + O(g_0^6)$. Once again, the first unknown contribution is at two-loop level: see [8] and [9] 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,

$$U_k(n)|_{n_0=0} \rightarrow W_k(\vec{n}) , \quad U_k(n)|_{n_0=T} \rightarrow W_k'(\vec{n}) \quad (k = 1, 2, 3),$$

(2.4)

for the gauge degrees of freedom\(^4\) and $(P_\pm = (\mathbb{I} \pm \gamma_5)/2$ with $\mathbb{I}$ being the identity matrix)

$$\psi^f(n)|_{n_0=0} \rightarrow \rho^f(\vec{n}) = P_+ \psi^f(n)|_{n_0=0} , \quad \psi^f(n)|_{n_0=T} \rightarrow \rho^f(\vec{n}) = P_+ \psi^f(n)|_{n_0=T} ;$$

(2.5)

$$\overline{\psi}^f(n)|_{n_0=0} \rightarrow \overline{\rho}^f(\vec{n}) = P_+ \overline{\psi}^f(n)|_{n_0=0} , \quad \overline{\psi}^f(n)|_{n_0=T} \rightarrow \overline{\rho}^f(\vec{n}) = P_+ \overline{\psi}^f(n)|_{n_0=T} ;$$

(2.6)

for fermions: boundary fields $W, W', \rho, \overline{\rho}, \rho'$ 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

$$S_G = \beta \sum_{n, \mu, \nu} \omega_{\mu\nu}(n) \left(1 - \frac{T_F}{2N_c} [U_{\mu\nu}(n) + U_{\mu\nu}^+(n)]\right),$$

(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 $e^{i\theta_\mu/L_F}$ 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

$$U_\mu(n) \rightarrow e^{i\theta_\mu/L_F} U_\mu(n),$$

(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 $W = \mathcal{P} e^{iC}$ and $W = \mathcal{P} e^{iC'}$ - see section 6 of [8] 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 $\mathcal{O}$ appearing in Eq.(2.3): a convenient choice reads,

$$\mathcal{O} = a^b \sum_{f,g} \sum_{\vec{m},\vec{n}} \bar{\zeta}^f(\vec{m}) \rho_{f,g} \frac{1}{2} \tau_f^b \zeta^g(\vec{m})^\prime,$$

(3.1)

where

$$\zeta^f(\vec{m}) = \frac{\delta}{\delta \bar{p}_f^f(\vec{m})}, \quad \bar{\zeta}^f(\vec{m}) = -\frac{\delta}{\delta \rho_f^f(\vec{m})}.$$

(3.2)

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

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

(3.3)

with

$$f_A = \frac{1}{12} \sum_{\vec{m},\vec{n}} \langle H^{ab}_{\vec{m}+\hat{0}} \omega_c, n \epsilon \delta \rangle \langle \eta_0 \rangle_{\vec{m}} \bar{\tau}^b_{f,g} \langle p \rangle_{\omega \sigma} \bar{J}_{\vec{m}+\hat{0}}^{gh} \tau_h \rangle_G,$$

(3.4)

$$f_p = \frac{1}{12} \sum_{\vec{m},\vec{n}} \langle H^{ab}_{\vec{m}+\hat{0}} \omega_c, n \epsilon \delta \rangle \langle \eta_0 \rangle_{\vec{m}} \bar{\tau}^b_{f,g} \langle p \rangle_{\omega \sigma} \bar{J}_{\vec{m}+\hat{0}}^{gh} \tau_h \rangle_G,$$

(3.5)

with

$$H^{if}_{\vec{m}+\hat{0}} = \left[ U_0(\vec{m}) \right]_{cb} \left( \tilde{M}^{-1} \right)^{if}_{\vec{m}+\hat{0}, \omega \epsilon \delta},$$

(3.6)

$$J^{gh}_{\vec{m}+\hat{0}} = \left[ U_0(\vec{m}) \right]_{cd} \left( \tilde{M}^{-1} \right)^{gh}_{\vec{m}+\hat{0}, \sigma \epsilon \delta},$$

(3.7)

where $\tilde{M}$ is the overall fermionic operator in the lattice action.

$f_A$, $f_p$ and $m_q$ depend on the lattice spacing $a$, the lattice extents $L_\mu$, the bare coupling $g_0$, the gauge fields $W$ and $W'$, the angles $\theta_0$ (from now on, we will set the latter equal to a common value $\theta$) and the improvement coefficient: recalling that the approach is perturbative, we can write

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

(3.8)

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.

We make the dependence on $W$, $W'$, $c_{SW}$ and $q_4$ 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.
and in turn, thanks to dimensional analysis

\[ m_q^{(k)}(L, \theta, x_0, a) = d_L(c_{SW}^{(i \leq k)}, c_A^{(i \leq k)}) \frac{a}{L} + d_{x_0}(c_{SW}^{(i \leq k)}, c_A^{(i \leq k)}) \frac{a}{x_0} + d_\theta(c_{SW}^{(i \leq k)}, c_A^{(i \leq k)}) \frac{a \theta}{L} + O(a^2). \tag{3.9} \]

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 \( d(c_{SW}^{(i \leq k)}, c_A^{(i \leq k)}) \) 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 \( c_{SW}^{(0)}, c_A^{(0)} \) and \( c_A^{(1)} \) to their known values; 2) perform simulations for different lattice extents keeping \( \theta, W \) and \( W' \) constant; 3) fit the coefficient \( d(c_{SW}, c_A^{(2)}) \); 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 \( \tilde{M}_0 \) appearing in \( S_F \); however, in the present setup, \textit{this is the case only if} \( \theta = 0 \): we chose to set \( \tilde{M}_0 = 0 \) but to work with non-vanishing \( \theta \) to avoid any infrared divergence.

Second, in Eq.(3.9) it is understood that mass counterterms - depending on \( c_{SW} \) - 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 [8]) 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 \textit{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 \( f_D \) eventually: to answer both, we must introduce some basics of NSPT.

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

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

where \( t \) is an extra degree of freedom (which can be thought as a \textit{stochastic time}), \( S \) is the part of the lattice action depending on the \( U' \)'s, \( \eta \) is a Gaussian noise while \( \nabla \) stands for the group derivative.

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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),

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

where \( T^A \) are the generators of the algebra and \( \mathcal{F} \) 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

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

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

Perturbation theory enters into play by \textit{formally} expanding each gauge degree of freedom in powers of \( \beta_0^{-1} \) - defined as \( \beta_0 = 2N_c/s_0^2 \) being \( N_c \) the number of colours - up to a given order \( s \) as

\[ U_\mu(n, t) = \mathbb{I} + \sum_{k=1}^{s} \beta_0^{-k} U^{(k)}_\mu(n, t), \tag{4.4} \]

and then plugging this Taylor series\(^9\) into Eq.(4.1): this results in a consistent \textit{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

\[
\begin{align*}
\tilde{M}^{-1(0)} &= \tilde{M}^{(0)}^{-1}, \\
\tilde{M}^{-1(1)} &= -\tilde{M}^{(0)}^{-1} \tilde{M}^{(1)} \tilde{M}^{(0)}^{-1}, \\
\tilde{M}^{-1(2)} &= -\tilde{M}^{(0)}^{-1} \tilde{M}^{(2)} \tilde{M}^{(0)}^{-1} + \\
&\quad -\tilde{M}^{(0)}^{-1} \tilde{M}^{(1)} \tilde{M}^{(1)} \tilde{M}^{(0)}^{-1}, \\
&\quad \ldots
\end{align*}
\]

where only the zeroth order of \( \tilde{M} \) has to be truly inverted: its expression for trivial \( W \) and \( W' \) can be found in section 3.1 of \[3\].

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 \( \theta \) and \( c_{SW}^{(0)} \)\(^11\) and compared the results

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\(^9\)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 \textit{background field} is introduced, the expansion would read \( U_\mu(n, t) = \exp[i(C_k - C_0)/T] \cdot [\mathbb{I} + \sum_k \beta^{-k} U^{(k)}_\mu(n, t)] \) - consult section 6.2 in \[3\] for the meaning of the first term in this product.

\(^10\)This relation is true only for continuous \( \tau \) so that simulations with different \( \tau \) 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.

| $\theta$ | $c_{SW}^{(0)} = 0.0$ | $c_{SW}^{(0)} = 1.0$ | $c_{SW}^{(0)} = 1.5$ |
|---|---|---|---|
| 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 $10^3 \times 21$ 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 $\theta$ ($m_q^{(0)}$ approaches with decreasing $\theta$ 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 $\tau$ 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 [3].