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On reweighting for twisted boundary conditions

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ABSTRACT

We consider the possibility of using reweighting techniques in order to correct the breaking of unitarity when twisted boundary conditions are imposed on valence fermions in simulations of lattice gauge theories. We start by studying the properties of reweighting factors and their variances at tree-level. This leads us to the introduction of a factorization for the fermionic reweighting determinant. In the numerical, stochastic implementation of the method, we find that the effect of reweighting is negligible in the case of large volumes but it is sizeable when the volumes are small and the twisting angles are large. More importantly, we find that for un-improved Wilson fermions, and in small volumes, the dependence of the critical quark mass on the twisting angle is quite pronounced and results in large violations of the continuum dispersion relation.

1. Introduction

Simulations of field theories on discretized Euclidean lattices are necessarily performed in a finite space–time volume. This requires imposing boundary conditions on the fields and although different choices have the correct infinite volume limit, the way that is approached depends on the particular choice (see for example the discussion in [1,2] for the case of lattice QED). The actual setup may affect not only the physical results by finite volume effects but also the algorithmic efficiency and sampling properties of the simulations. Recent examples of the latter can be found in [3] for the use of open boundary conditions in lattice QCD to bypass the freezing of topology, and in [4] for the use of generalized boundary conditions in order to exponentially improve the signal to noise ratio in glueball correlation functions computed in the pure gauge theory. When considering lattice QCD, (anti)-periodic boundary conditions in (time)-space are usually imposed on the fermionic fields. This leads to a quantization of the spatial momenta in units of $2\pi/L$ with L the spatial extent of the lattice. For the lowest non-zero momentum to be around 100 MeV, lattices of about 12 fm extension are needed. This is still very demanding from the computational point of view if at the same time one wants to keep discretization effects under control, which typically requires considering lattice spacings a of about 0.1 fm and below. In addition, for several applications relevant for phenomenology, it is desirable not only to reach small momenta, but also to have a fine resolution of them. Examples include form factors, as those describing the $K \to \pi \ell \nu$ transition, the charge radius of the pion, and the hadronic vacuum polarization of the photon, relevant for the muon $g-2$ anomaly.

Twisted boundary conditions, first introduced in [5,6] offer a way to continuously vary momenta in lattice QCD, and have indeed been used for all the computations mentioned above [7–9]. They have also been applied to the calculation of renormalization factors in the RI-MOM scheme [10] and to the matching between Heavy Quark Effective Theory and QCD using correlators defined in the Schrödinger Functional [11]. Twisting amounts to imposing periodic boundary conditions up to a phase (the twisting angle θ) for fermions in the spatial directions. In actual simulations, the partially twisted setup is usually adopted, where twisting is only applied in the valence sector whereas fermions in the sea are kept periodic. This introduces a breaking of unitarity as a boundary effect, which therefore is expected to disappear in the infinite volume limit, as it has explicitly been checked using Chiral Perturbation Theory in [12].

This suggests that reweighting techniques as those employed in [13] for the case of mass-reweighting could be used here in order to change the periodicity conditions for fermions in the sea. We will see in the following that the resulting reweighting factors are ratios of fermionic determinants, which tend to the value one in the infinite volume limit. Therefore, as mentioned above, if any effect of unitarity violations can be seen, then that is expected to happen in rather small volumes, where the reweighting factors (which are extensive quantities) can be reliably computed and used as correction factors if needed.

A preliminary account of the present studies appeared in [14]. The paper is organized as follows: in Section 2, we collect definitions and details on the setup we used; in Section 3, we present exact results obtained at tree-level. Those will turn out to be useful

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in optimizing the numerical techniques employed for the evaluation of the reweighting factors and their variances. Simulation parameters and Monte-Carlo results are presented in Section 4. The pion and quark mass dependence on the twisting angle are discussed in Section 5. Section 6 contains our conclusions.

2. Definitions and setup

The generic boundary conditions for matter fields in lattice QCD formulated on a torus are nicely discussed in [12]. There it is pointed out that it is sufficient to require that the action is single valued on the torus, whereas the fields themselves do not need to be. Periodicity conditions on the fermions can therefore be of the form

$$\Psi\left(x + L_\mu \hat{\mu}\right) = V_\mu \Psi\left(x\right)\ , \quad \mu = 1, 2, 3, \tag{2.1}$$

where Ψ is a flavor multiplet and V_μ represents a unitary transformation associated to a symmetry of the action. Similarly, for the $\overline{\Psi}$ field, one requires

$$\overline{\Psi}\left(x + L_\mu \hat{\mu}\right) = \overline{\Psi}\left(x\right) V_\mu^\dagger\ , \quad \mu = 1, 2, 3. \tag{2.2}$$

Considering now the generic values of the diagonal quark mass matrix, one concludes that V_μ also has to be diagonal in flavor space, i.e

$$\psi\left(x + L_\mu \hat{\mu}\right) = e^{i\theta_\mu} \psi\left(x\right)\ , \quad \mu = 1, 2, 3\,, \tag{2.3}$$

where the twisting angles $\theta_\mu \in [0, 2\pi)$ have been introduced for each flavor and ψ is now one component of the Ψ multiplet.

Equivalently, one can fix the fermionic fields to be periodic and introduce a constant U(1) interaction with vanishing electric and magnetic fields, vanishing electric potential but constant vector potential [6,12]. In lattice gauge theories, such an interaction is implemented by transforming the standard QCD links $U_\mu(x)$ in the following way (setting $a = 1$):

$$\tilde{U}_\mu(x) = \begin{cases} e^{i\theta_\mu/L_\mu} U_\mu(x)\ , & \mu = 1, 2, 3 \\ U_0(x)\ , & \mu = 0. \end{cases} \tag{2.4}$$

In order to see the equivalence, it is enough to observe that the phase can be re-absorbed by re-writing the, now periodic, ψ fields in terms of

$$\tilde{\psi}(x) = e^{i\overrightarrow{\left(\frac{\theta}{L}\right)}\vec{x}}\psi(x)\,, \tag{2.5}$$

and to notice that the $\tilde{\psi}$ are indeed periodic up to a phase, as for Eq. (2.3). The spatial Fourier modes of the $\langle\tilde{\psi}(x)\overline{\tilde{\psi}}(0)\rangle$ propagator are of the shifted form $e^{i\left(\vec{k}+\frac{\vec{\theta}}{L}\right)\vec{x}}$ with each component of the vector $\vec{k}$ being an integer multiple of $2\pi/L$ (for the special but rather typical case $L_1 = L_2 = L_3 = L$). In this sense, twisting allows to continuously vary momenta as mentioned in the introduction. The corresponding amplitudes can be extracted from the Fourier decomposition of the propagator $\langle\psi(x)\overline{\psi}(0)\rangle$, which satisfies periodic boundary conditions. In practice, SU(N_c) gauge configurations are typically produced for one specific choice of θ, and the angle is then varied only when computing the quark propagators, which is cheaper in terms of CPU-time with respect to the generation of configurations. As a consequence, the quark propagators in the sea and valence sectors differ, which causes a breaking of unitarity already at the perturbative level. This effect however can be studied in a rather straightforward way, as done here.

In the following, we will use the un-improved Wilson action, with the links $U_\mu(x)$ replaced by the $\tilde{U}_\mu(x)$ as in Eq. (2.4). This replacement clearly does not affect the plaquettes and therefore the pure gauge term in the action. Only the covariant derivatives and the Wilson term are modified. Hence, once the fermionic degrees of freedom are integrated out on each SU(N_c) gauge background, the θ-dependence from the sea sector is completely absorbed in the fermionic determinant.

In order to apply reweighting techniques, let us imagine we want to compute the value of some observables for one choice of bare parameters $B = \{\beta', m_1', m_2', \ldots, m_{n_f}', \theta_\mu', \ldots\}$, using the configurations produced at a slightly different set of parameters $A = \{\beta, m_1, m_2, \ldots, m_{n_f}, \theta_\mu, \ldots\}$. To this end, one needs to compute on each configuration of the A-ensemble the reweighting factor $W_{AB} = P_B/P_A$, which is the ratio of the two probability distributions and it is an extensive quantity, $P_A[U] = e^{-S_G[\beta,U]}\prod_{i=1}^{n_f}\det\left(D[U,\theta] + m_i\right)$. In the last expression, we have explicitly indicated the dependence of the Dirac operator on the twisting angle. The expectation values on the B-ensemble can then be expressed as

$$\langle\mathcal{O}\rangle_B = \frac{\langle\widetilde{\mathcal{O}}W_{AB}\rangle_A}{\langle W_{AB}\rangle_A}\,, \tag{2.6}$$

with $\widetilde{\mathcal{O}}$ being the observable defined after Wick contractions, and $\langle\ldots\rangle_A$ indicates that expectation values have to be taken on the A-ensemble. Specializing to the case where only the periodicity angles of the fermionic boundary conditions are changed from one bare set to the other, we obtain the following expression of the reweighting factor:

$$W_\theta = \det\left(D_W[U,\theta]D_W^{-1}[U,0]\right) = \det\left(D_W[\tilde{U},0]D_W^{-1}[U,0]\right), \tag{2.7}$$

where we have also chosen D to be D_W, i.e., the massive Wilson Dirac operator. Under certain conditions ratios of determinants as those above can be estimated stochastically. In general, for a normal matrix M whose eigenvalues have positive real parts, the following representation of the determinant can be used [13]:

$$\frac{1}{\det M} = \int \mathcal{D}[\eta]\exp\left(-\eta^\dagger M\eta\right) < \infty \iff \mathbb{R}\mathrm{e}\lambda\left(M\right) > 0. \tag{2.8}$$

The positivity condition ensures that the integral converges. The expression can clearly be evaluated stochastically. The distribution $p(\eta)$ of the vectors η is usually taken to be gaussian; in this case, the determinant (or its inverse) can be written as

$$\frac{1}{\det M} = \left\langle\frac{e^{-\eta^\dagger M\eta}}{p(\eta)}\right\rangle_{p(\eta)} = \frac{1}{N_\eta}\sum_{k=0}^{N_\eta} e^{-\eta_k^\dagger(M-\mathbf{1})\eta_k} + O\left(\frac{1}{\sqrt{N_\eta}}\right). \tag{2.9}$$

It is straightforward to generalize the positivity condition above in order to ensure the convergence of the stochastic estimates of all Gaussian moments. In the case of an Hermitian matrix, one obtains

$$\left\langle\frac{e^{-2\eta^\dagger M\eta}}{p(\eta)^2}\right\rangle_{p(\eta)} = \int\mathcal{D}[\eta]\exp\left[-\eta^\dagger(2M-\mathbf{1})\eta\right] < \infty$$
$$\iff \lambda\left(M\right) > \frac{1}{2},$$
$$\vdots$$
$$\left\langle\frac{e^{-N\eta^\dagger M\eta}}{p(\eta)^N}\right\rangle_{p(\eta)} = \int\mathcal{D}[\eta]\exp\left[-\eta^\dagger[NM-(N-1)\mathbf{1}]\eta\right] < \infty$$
$$\iff \lambda\left(M\right) > \frac{N-1}{N}\underset{N\to\infty}{\longrightarrow} 1.$$

All eigenvalues should therefore be larger than unity. In particular, in the numerical studies presented here, we will always consider the square of the Hermitian version of the Wilson Dirac operator $Q = \gamma_5 D_W$, which is to say we consider the case of two degenerate flavors.

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