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Twisted boundary conditions in lattice simulations

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Abstract

By imposing twisted boundary conditions on quark fields it is possible to access components of momenta other than integer multiples of $2\pi/L$ on a lattice with spatial volume L^3. We use chiral perturbation theory to study finite-volume effects with twisted boundary conditions for quantities without final-state interactions, such as meson masses, decay constants and semileptonic form factors, and confirm that they remain exponentially small with the volume. We show that this is also the case for *partially twisted* boundary conditions, in which (some of) the valence quarks satisfy twisted boundary conditions but the sea quarks satisfy periodic boundary conditions. This observation implies that it is not necessary to generate new gluon configurations for every choice of the twist angle, making the method much more practicable. For $K \to \pi\pi$ decays we show that the breaking of isospin symmetry by the twisted boundary conditions implies that the amplitudes cannot be determined in general (on this point we disagree with a recent claim).

1. Introduction

In lattice simulations of QCD on a cubic volume ($V = L^3$) with periodic boundary conditions imposed on the fields, the hadronic momenta (p) are quantized according to $p_i = 2\pi/L \times n_i$, where $i = 1, 2, 3$ and the n_i are integers. For currently available lattices this means that the lowest non-zero momentum is large (typically about 500 MeV or so) and there are big gaps between neighbouring momenta. This limits the phenomenological reach of the simulations. In Ref. [1] Bedaque proposed the use of non-periodic boundary conditions which would allow hadrons with arbitrarily small momenta to be simulated (see also the references cited in [1] for earlier related ideas). We refer to these boundary conditions as *twisted* boundary conditions.[1] This technique has subsequently

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[1] An analogous method was already introduced many years ago in the context of extra-dimensions [2] and is still widely used for breaking spontaneously some of the action symmetries. The breaking is spontaneous since it is caused by a non-local effect.

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been used in a quenched study of the energy–momentum dispersion relations of pseudoscalar mesons [3] and the finite-volume corrections for two-particle states with twisted boundary conditions have been calculated [4].

In this Letter we use chiral perturbation theory (χPT) to analyse some of the properties of twisted boundary conditions and show that:

(1) For physical quantities without final state interactions, such as masses or matrix elements of local operators between states consisting of the vacuum or a single hadron, the flavour symmetry breaking induced by the twist only affects the finite-volume corrections, which nevertheless remain exponentially small;

(2) For amplitudes which involve final-state interactions, such as those for $K \to \pi\pi$ decays, in general it is not possible to extract the physical matrix elements using twisted boundary conditions (see Section 4). On this point we disagree with Ref. [4];

(3) For *partially twisted* boundary conditions, in which (some of) the valence quarks satisfy twisted boundary conditions but the sea quarks satisfy periodic ones, one also obtains the physical quantities described in item (1) with exponential precision in the volume. This implies that in unquenched simulations it is not necessary to generate new gluon configurations for every choice of boundary condition, thus making the method much more practicable.

In Ref. [5] Kim and Christ propose H- and G-parity boundary conditions in which the minimum non-zero hadronic momenta are reduced from $2\pi/L \to \pi/L$ (see also Ref. [6]). These authors impose H-parity boundary conditions for $K \to \pi\pi$ decays in which the two-pions are in an $I = 2$ state. This is a particular case of twisted boundary conditions, corresponding to the specific choice of π for the twisting angle (as stated in item (2) above and explained in Section 4 below, it is not possible to study $K \to \pi\pi$ decays with a general choice of twisting angle). Kim and Christ also show that G-parity boundary conditions, which exploit the discrete charge conjugation transformations, can be used for an $I = 0$ two-pion state (in unquenched simulations), but the formalism will have to be extended to incorporate the kaon. Although we do comment below on H- and G-parity boundary conditions in order to illustrate our discussion, the main focus of this Letter is on boundary conditions based on continuous symmetries.

When considering $K \to \pi\pi$ decays, throughout this Letter we restrict our discussion to the centre-of-mass frame for the two pions. For this case and with periodic boundary conditions, the finite-volume corrections which decrease as powers of the volume have been derived for the two-pion spectrum [7] and matrix elements [8,9]. At present the theory of finite-volume corrections in a moving frame has not been developed for matrix elements (but for a discussion of finite-volume corrections to the two-pion spectrum in a moving frame see Ref. [10]). We therefore do not generalise our discussion to the moving frame at this stage.

The plan of the remainder of this Letter is as follows. In the following section we define twisted boundary conditions in QCD and briefly review their properties. In Section 3 we impose twisted boundary conditions on the chiral Lagrangian and demonstrate that their effect is to shift the momenta of internal propagators and external mesons by amounts corresponding to the twists. Section 4 contains a discussion of finite-volume effects when twisted boundary conditions have been imposed. We discuss partially twisted boundary conditions in Section 5 and present our conclusions in Section 6. There are two appendices in which we derive the finite-volume corrections with twisted boundary conditions at one-loop order in χPT (Appendix A) and present the corresponding results for meson masses and decay constants (Appendix B).

2. Twisted boundary conditions in QCD

In this section we will define the twisted boundary conditions and derive some of the constraints they have to satisfy. Since the choice of boundary conditions is a non-local effect, we can present the discussion, without any loss of generality, within the framework of continuum quantum field theory. It should be noted however, that the discussion also applies to every lattice discretization. Although local discretization artefacts may affect the constant