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Finite-volume two-pion amplitudes in the $I = 0$ channel

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Abstract

We perform a calculation in one-loop chiral perturbation theory of the two-pion matrix elements and correlation functions of an $I = 0$ scalar operator, in finite and infinite volumes for both full and quenched QCD. We show that major difficulties arise in the quenched theory due to the lack of unitarity. Similar problems are expected for quenched lattice calculations of $K \rightarrow \pi\pi$ amplitudes with $\Delta I = 1/2$. Our results raise the important question of whether it is consistent to study $K \rightarrow \pi\pi$ amplitudes beyond leading order in chiral perturbation theory in quenched or partially quenched QCD.

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1. Introduction

A precise quantitative evaluation of weak non-leptonic amplitudes in kaon decays is an enormous challenge for lattice QCD. Although it has been demonstrated that such a calculation is possible, in principle, a number of major practical difficulties must first be overcome. These difficulties are related to the construction of finite matrix elements of renormalized operators from the lattice bare ones and to the extraction of physical amplitudes, including final state interaction phases, from Euclidean correlation functions. For the latter problem, it has been demonstrated that it would be possible in principle to obtain the physical amplitudes by performing unquenched simulations with physical quark masses on lattice volumes large enough to have discretization errors and finite size effects under control [1,2]. At present, however, it is not possible to perform unquenched simulations on such large volumes and therefore a certain number of approximations are necessary. One of the main approximations (in addition to quenching) consists in working with unphysical quark masses and/or external meson momenta, and estimating the physical amplitudes by extrapolating to the physical point. A key element of our strategy in evaluating $K \rightarrow \pi\pi$ matrix elements is the use of Chiral Perturbation Theory (χ PT) at next-to-leading order (NLO) [3]. In a recent paper [4], we have presented the relevant formulae for $\Delta I = 3/2$ transitions on finite and infinite volumes, in the full theory and in the quenched approximation. Our results show explicitly that all corrections which vanish as

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inverse powers of the volume can be eliminated by using the methods introduced in Refs. [1,2].¹ The remaining finite volume corrections are exponentially small (of $\mathcal{O}(e^{-mL})$). At the NLO in χ PT this is true also in the quenched approximation.

In this Letter we present the results obtained at NLO in χ PT for matrix elements with an $I = 0$ two-pion final state. We study these matrix elements in order to illustrate the main features present in $\Delta I = 1/2$ $K \rightarrow \pi\pi$ transitions in quenched QCD. For these decays, the lack of unitarity of the quenched theory leads to a number of problems which need to be solved in order to understand the volume dependence and to extract the amplitudes. The main consequences of quenching, due to the lack of unitarity, can be summarized as follows:

- the final state interaction phase is not universal, since it depends on the operator used to create the two-pion state. This is not surprising, since the basis of Watson's theorem is unitarity;
- the Lüscher quantization condition [6] for the two-pion energy levels in a finite volume does not hold;
- a related consequence is that the Lellouch–Lüscher (LL) relation between the absolute value of the physical amplitudes and the finite volume matrix elements [1,2] is no longer valid. It is, therefore, not possible to take the infinite volume limit at constant physics, namely, with a fixed value of W ;
- whereas it is normally possible to extract the lattice amplitudes by constructing suitable time-independent ratios of correlation functions, this procedure fails in the quenched theory as explained in Section 2.2. In particular, the time dependence of correlation functions corresponding to different operators which create the same external state is not the same;
- in addition to the usual exponential dependence on the time intervals, the presence of the double pole corresponding to the incomplete η' propagator generates, at one-loop order in χ PT, terms in the Euclidean correlation functions which depend linearly, quadratically or cubically on the time [7]. Unlike the corrections which shift the two-pion energy in a finite volume [4], these terms do not exponentiate and may cause practical problems in the extraction of the finite volume matrix elements. A related problem is the appearance, at fixed L , of corrections linear or cubic in L [7,8].

The last problem can be overcome by working in partially quenched QCD, where the η' is heavy and decouples from the light Goldstone boson sector. All the problems originating from the lack of unitarity (denoted as the *unitarity problem* in the following) would, however, remain the same. Unitarity is recovered from partially quenched QCD only in the limit when the number of sea and valence quarks is equal and their masses are equal. This corresponds to full QCD.

In view of the difficulties listed above, it may be questioned whether it is possible to obtain $K \rightarrow \pi\pi$ decay amplitudes beyond leading order in χ PT in quenched or partially quenched QCD. In the absence of a solution to the problems encountered and discussed in this Letter, we would be limited to extracting the effective couplings (the low-energy constants) corresponding to the operators in the weak Hamiltonian at lowest order in the chiral expansion from $K \rightarrow \pi$ matrix elements computed in lattice simulations. The absence of unitarity is intrinsic to quenched and partially quenched QCD, and we do not have a solution to the unitarity problem. Nevertheless it is tempting to speculate whether there might not be a possible pragmatic way to proceed, in spite of the failure of Watson's theorem. Indeed the key point is that, in the quenched case, the two-pion state is no longer an eigenstate of the strong interaction Hamiltonian. The eigenstates of the Hamiltonian would be, formally, linear combinations of physical pions and unphysical mesons composed of the pseudo-fermion fields. The latter, however, have the wrong spin-statistic properties and for this reason unitarity breaks down. We speculate that it might be possible to recover a variation of Watson's theorem, and of the LL formula in finite volumes, by a suitable reinterpretation of the quenched theory, for example, by using the replica method of Ref. [5], working in the basis of Hamiltonian

¹ The infinite-volume limit, $L \rightarrow \infty$ (where L is the length of each spatial dimension of the lattice), is to be taken at fixed physics, i.e., at fixed two-pion energy W .

eigenstates. However, we stress that this is only a speculation and we will report on the conclusions of our investigations of this important question in a future paper.

Since all the major difficulties arising from the *unitarity problem* depend only on the quantum numbers of the operators and final state, for the sake of illustration we discuss in this Letter matrix elements of the form $\langle \pi\pi | S | 0 \rangle$, where S is a scalar and isoscalar operator which can annihilate the two-pion state. We also discuss the properties of the correlation functions from which such matrix elements are obtained. The discussion can readily be extended to $K \rightarrow \pi\pi$ matrix elements of $\Delta I = 1/2$ operators of the effective weak Hamiltonian [9]. The results for the $\Delta I = 1/2$ amplitudes in one loop χ PT on finite and infinite volumes, in the full theory and in the quenched approximation, will be presented in a forthcoming publication [10]. In our calculation we have used the formulation of the quenched chiral Lagrangian introduced in Ref. [11], using the conventions and notation presented in Section 3 of Ref. [4]. The scalar operator is defined by

$$S = \text{tr}[\Sigma + \Sigma^\dagger], \quad (1)$$

in the full theory and as

$$S^q = \sum_{i=1,3} [\Sigma^q + \Sigma^{q\dagger}]_{ii}, \quad (2)$$

in the quenched theory, where the trace (sum) is taken over the indices of the chiral group $SU(3)_L \otimes SU(3)_R$ (graded group $SU(3|3)_L \otimes SU(3|3)_R$). In the quenched case the field Σ^q is the graded extension of the standard field Σ of the full theory.

The main results of our calculations are presented in Appendices A–D, which contain the following:

- (1) the NLO expression for the matrix element of the scalar operator in full QCD and in infinite volume, $\langle \pi^+ \pi^- | S | 0 \rangle$. This is given in Eq. (A.2);
- (2) the expression for the corresponding quantity in the quenched theory $\langle \pi^+ \pi^- | S^q | 0 \rangle$, presented in Eq. (B.2);
- (3) the NLO result for the correlation function $\langle 0 | \pi_{-\bar{q}}^+(t_1) \pi_{\bar{q}}^-(t_2) S(0) | 0 \rangle$ in a finite volume and in full QCD. This is given in Eq. (C.1);
- (4) the corresponding correlation function in the quenched theory, $\langle 0 | \pi_{-\bar{q}}^+(t_1) \pi_{\bar{q}}^-(t_2) S^q(0) | 0 \rangle$, presented in Eq. (D.1).

In the above $S(0) \equiv S(\vec{x} = 0, t = 0)$ with the corresponding definition of $S^q(0)$. The expressions for the matrix elements are given in Minkowski space, whereas those for the correlation functions are presented in Euclidean space. In the correlation functions we have used the following definition for the Fourier transform of the fields

$$\pi_{\bar{q}}(t) = \int d^3x \pi(\vec{x}, t) e^{i\vec{q}\cdot\vec{x}}. \quad (3)$$

The correlation functions depend on the choice of t_1 and t_2 . In this Letter, for purposes of illustration, we present the results for the two cases $t_1 = t_2$ and $t_1 \gg t_2$.

In Section 2 we discuss the physical interpretation of the expressions obtained at one-loop in χ PT for the different cases and the implications for the relation between finite volume Euclidean correlation functions and physical amplitudes (including final state interaction phases) [1,2]. The relevant expressions and the technical details can be found in the appendices.

2. Discussion of the one-loop calculations

In this section, we discuss the extraction of the physical amplitudes from finite-volume Euclidean correlation functions, using the results obtained in one-loop χ PT. We first consider the unquenched case, where we explicitly check the validity of LL relation [1,2], derived using general properties of quantum mechanics and field theory.

2.1. Extraction of the physical amplitude from the scalar correlation function in full QCD

We begin our discussion from the correlation function of the scalar operator with two pion fields, in the full theory at finite volume, $\langle 0 | \pi_{-\vec{q}}^+(t_1) \pi_{\vec{q}}^-(t_2) S(0) | 0 \rangle$. The tree-level and one-loop diagrams are shown in Figs. 1(t) and (z), (a) and (b). Final state interactions, and consequently power-like finite volume corrections, are only given by the diagram in Fig. 1(b).² The NLO expression for the correlation function is given in Eq. (C.1). The corresponding Minkowski amplitude in infinite volume is given in Eq. (A.2). In this case we denote the contribution of the diagrams in Figs. 1(z), (a) and (b) by I_z , I_a and I_b , respectively, and define the relative one-loop correction to the infinite volume amplitude as $\mathcal{A}_\infty = 1/(4\pi f)^2 (I_z + I_a + I_b)$, see Eqs. (A.2) and (A.3). Final state interactions are encoded in the function $A(m)$ introduced in Eq. (A.4).

In a finite volume the corrections to the amplitude from the diagrams in Figs. 1(z) and (a) (I_z and I_a , respectively) are the same as in infinite volume up to exponentially small terms (in the volume) that will be neglected in the following. The diagram in Fig. 1(b) gives a correction, $I_b(t_1, t_2)$, which is a function of the time coordinates of the interpolating operators which annihilate the two pions (the two-pion sink).

At lowest order (obtained by setting $I_z = I_a = I_b(t_1, t_2) = 0$), the time dependent factor

$$\frac{e^{-Et_1}}{2E} \frac{e^{-Et_2}}{2E}, \quad (4)$$

can be removed by dividing by the two-pion propagator in the free theory, and in this way the required matrix element can be obtained. In Eq. (4) E is the energy of each of the pions, $E = \sqrt{\vec{q}^2 + m_\pi^2}$.

At one-loop order the relevant finite-volume correction to the correlation function of Eq. (C.1) is, therefore, given by $I_b(t_1, t_2)$ which is presented explicitly in Eq. (C.2). We rewrite $I_b(t_1, t_2)$ as $I_b(t_1, t_2) = \text{Re}(I_b) + \mathcal{T}(t_2) + \mathcal{R}(t_1, t_2)$, where I_b is the corresponding infinite-volume one-loop contribution to the matrix element (see Eq. (A.3)) and we now discuss the significance of the terms \mathcal{T} and \mathcal{R} .

$\mathcal{T}(t_2)$ contains the one-loop corrections which are multiplied by the *correct* time dependence, $\exp(-Wt_2) \exp(-E(t_1 - t_2))$ (after exponentiation), where $W = 2E + \Delta W$ and ΔW is the shift of the two-pion energy due to interactions in the finite volume [4]. We can readily extract ΔW from the coefficient of t_2 in the expression for

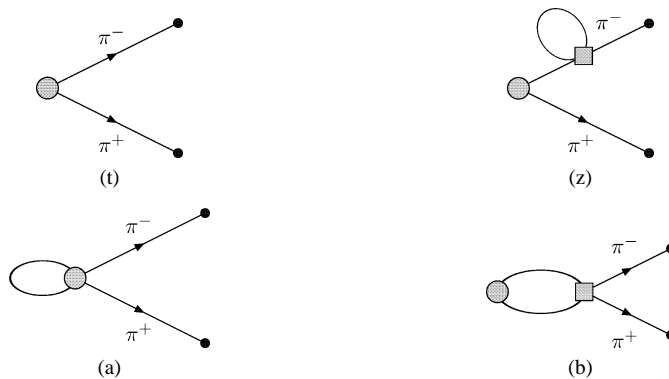


Fig. 1. Tree level (t) and one-loop χ PT diagrams for the $\langle \pi^- \pi^+ | S | 0 \rangle$ amplitude and $\langle 0 | \pi^- \pi^+ S | 0 \rangle$ correlation function. The grey circle represents the scalar source while the squares are strong vertices.

² The evaluation of this diagram for $I = 2$ final states was explained in some detail in Section 4 of Ref. [4]. We therefore do not present a description of the calculation for $I = 0$ final states, but limit the discussion to the implications of the results.

$\mathcal{T}(t_2)$ in Eq. (C.4),

$$\Delta W = -\frac{\nu}{4f^2L^3} \left(8 - \frac{m_\pi^2}{E^2} \right). \quad (5)$$

It is then straightforward to check that Eq. (5) reproduces the well known result for the scattering length $a_0^{I=0}$ [13]. When the two pions are at rest Eq. (5) gives

$$W = 2m_\pi - \frac{4\pi a_0^{I=0}}{m_\pi L^3}, \quad (6)$$

where $a_0^{I=0} = 7m_\pi / (16\pi f_\pi^2)$.

$\mathcal{T}(t_2)$ also contains the finite volume corrections to:

- (1) the matrix element of the scalar operator. These are given by the one-loop component of the LL-factor relating the infinite-volume and finite-volume amplitudes, \mathcal{M}_∞ and \mathcal{M}_V , respectively, ($|\mathcal{M}_\infty|^2 = LL \times |\mathcal{M}_V|^2$);
- (2) the two-pion sink used to annihilate the pions created by the scalar source. We refer to these as *Forward Time Contributions* or FTCs. They are presented explicitly in Eq. (C.6).

The FTCs are eliminated by dividing $\langle 0 | \pi_{-\vec{q}}^+(t_1) \pi_{\vec{q}}^-(t_2) S(0) | 0 \rangle$ by (the square root of) a suitable $\pi\pi$ correlation function [4]

$$\begin{aligned} G_{\pi\pi \rightarrow \pi\pi}(t_1, t_2) &\equiv \sum_{\vec{p}, \vec{q}; |\vec{p}|=|\vec{q}|, |\vec{q}| \text{ fixed}} \langle 0 | \pi_{\vec{q}}(t_1) \pi_{-\vec{q}}(t_2) \pi_{-\vec{p}}^\dagger(-t_2) \pi_{\vec{p}}^\dagger(-t_1) | 0 \rangle \\ &= \nu \frac{e^{-2Wt_2}}{(2E)^2} L^6 \left(1 + \left(1 - \frac{3m_\pi^2}{8E^2} \right) \frac{2\nu}{3f^2EL^3} \right), \quad \text{for } t_1 = t_2, \\ &= \nu \frac{e^{-2Wt_2 - 2E(t_1 - t_2)}}{(2E)^2} L^6 \left(1 + \left(1 - \frac{3m_\pi^2}{8E^2} \right) \frac{\nu}{3f^2EL^3} \right), \quad \text{for } t_1 \gg t_2. \end{aligned} \quad (7)$$

Note that in the unquenched case the finite-volume energy W appearing in Eq. (7) is, as expected, the same as in

$$\langle 0 | \pi_{-\vec{q}}^+(t_1) \pi_{\vec{q}}^-(t_2) S(0) | 0 \rangle \propto e^{-E(t_1 - t_2)} e^{-Wt_2}, \quad (8)$$

because we are considering the same final state. As shown below, this is not true in the quenched and in the partially quenched theories.

Finally $\mathcal{R}(t_1, t_2)$ corresponds to contributions to the correlation function whose time dependence is governed by energies different from W and which therefore can be eliminated by studying this time dependence [4,12]. Since it is not relevant to our discussion, $\mathcal{R}(t_1, t_2)$ will be neglected in the formulae given in the appendices.

2.2. The scalar correlation function in the quenched theory

In one-loop χ PT with $I = 2$ final states (as, for example, in $\Delta I = 3/2$ $K \rightarrow \pi\pi$ transitions) we can follow the path outlined above for full QCD also in the quenched theory. This is not the case, however, when we consider the infinite-volume amplitude or the finite-volume correlation function of the isosinglet scalar operator with two pion fields in the quenched theory. The one-loop expression for the amplitude $\langle \pi^+ \pi^- | S^q | 0 \rangle$ is given in Eq. (B.2) and for the correlation function $\langle 0 | \pi_{-\vec{q}}^+(t_1) \pi_{\vec{q}}^-(t_2) S^q(0) | 0 \rangle$ in Eq. (D.1). In this case, even in infinite volume there are severe difficulties, for example, the imaginary part of the amplitude given in Eq. (B.2), corresponding to the final state interactions, depends on the scalar operator and diverges at threshold, i.e., when $s \rightarrow 4m_\pi^2$ [15]. We now consider what happens for the correlation function in a finite volume.

For illustration, let us start by neglecting the contribution of the η' double pole by setting $m_0 = 0$ and $\alpha = 0$ (they are defined in Eq. (B.1)). For simplicity we also neglect the terms proportional to $v_{1,2}$ ($v_{1,2}$ are also defined

in Eq. (B.1)). This is similar to the situation encountered in the partially quenched case where the η' is heavy, but unitarity is violated. In this case all the $a_{11}^{(i)}$ defined in Appendix D satisfy $a_{11}^{(i)} = 0$ and for $E < m_K < m_{\bar{s}s}$ only the first line of $\mathcal{T}^q(t_2)$ in Eq. (D.4) contributes

$$\mathcal{T}^q(t_2) = -\frac{E^2}{2f^2} \left[-\frac{2vt_2}{E^2L^3} + \left(-\frac{v}{3E^3L^3}; -\frac{v}{6E^3L^3} \right) + \left(\frac{z(0)}{2E^3L^3} - \frac{z(1)}{2\pi^2EL} \right) \right]. \quad (9)$$

The terms $(\dots; \dots)$ are the forward-time contributions (FTCs) respectively, for the two cases $t_1 \gg t_2$ and $t_2 = t_1$.

The first term in Eq. (9) is the shift in the energy of the two-pion final state. This shift,

$$\Delta W = -\frac{v}{f^2L^3} \quad (10)$$

is different from that obtained from the $\pi\pi \rightarrow \pi\pi$ correlation function in Eq. (7), which is

$$\Delta W = -\frac{v}{4f^2L^3} \left(8 - \frac{m_\pi^2}{E^2} \right). \quad (11)$$

The latter in fact is the same in the quenched and unquenched theories, since, at this order, it is given by a tree diagram. Once the contribution from the η' double pole is included, at this order there are quadratic and cubic terms in t_2 present in $\mathcal{T}^q(t_2)$, but not in the $\pi\pi \rightarrow \pi\pi$ correlation function.

The second term in Eq. (9) should be cancelled when extracting the matrix element of the scalar operator by dividing by the square root of the $\pi\pi \rightarrow \pi\pi$ correlation function:

$$|\langle \pi\pi | S^q | 0 \rangle_V| = \frac{\langle 0 | \pi_{-\bar{q}}^+(t_1) \pi_{\bar{q}}^-(t_2) S^q(0) | 0 \rangle}{\sqrt{G_{\pi\pi \rightarrow \pi\pi}(t_1, t_2)}}, \quad (12)$$

since it is the finite volume correction to the sink operator used to annihilate the two pions. One can readily verify that the cancellation does not occur, unlike in the unquenched theory. Thus the power corrections in $1/L$ to $|\langle \pi\pi | S^q | 0 \rangle_V|$ are not those expected on the basis of the Lellouch–Lüscher formula.

3. Conclusion

In this Letter we have shown that the standard strategy for extracting the amplitude and the relative phase from finite-volume calculations of correlation functions fails in the quenched theory for $I = 0$ two-pion final states. We encounter the same problems when computing the matrix elements of the operators relevant for $\Delta I = 1/2$ $K \rightarrow \pi\pi$ transitions at one-loop order in χ PT [10].

At present we do not know whether it might be possible to recover a modification of Watson's theorem and of the LL formula in finite volumes, which would allow for a consistent determination of $I = 0$ two-pion matrix elements beyond leading order in quenched χ PT. We are currently investigating the possibility of performing a suitable analytic continuation in the numbers of flavours, using the replica method of Ref. [5] at one-loop order in χ PT.

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Appendix A. The scalar amplitude in full QCD

To fix the conventions we start by writing the chiral Lagrangian used in our calculations in the full QCD:

$$\mathcal{L}_{\text{strong}} = \frac{f^2}{8} \text{tr} \left[(\partial_\mu \Sigma^\dagger) (\partial^\mu \Sigma) + \Sigma^\dagger \chi + \chi^\dagger \Sigma \right], \quad (\text{A.1})$$

where the decay constant f is normalized in such way that $f_\pi \sim 132$ MeV.

The one-loop matrix element of the scalar operator in full QCD in infinite volume is given by

$$\langle \pi^-(\vec{q}) \pi^+(-\vec{q}) | S | 0 \rangle \equiv -\frac{8}{f^2} [1 + \mathcal{A}_\infty] = -\frac{8}{f^2} \left[1 + \frac{1}{(4\pi f)^2} (I_z + I_a + I_b) \right], \quad (\text{A.2})$$

where

$$\begin{aligned} I_z &= -\frac{2}{3} m_K^2 \log\left(\frac{m_\pi^2}{m_K^2}\right) + \frac{2}{3} (m_K^2 + 2m_\pi^2) \log\left(\frac{m_\pi^2}{\mu^2}\right), \\ I_a &= -\frac{m_\eta^2}{3} \log\left(\frac{m_\eta^2}{\mu^2}\right) - \frac{5m_\pi^2}{3} \log\left(\frac{m_\pi^2}{\mu^2}\right) - \frac{4m_K^2}{3} \log\left(\frac{m_K^2}{\mu^2}\right), \\ I_b &= (m_\pi^2 - 2s) A(m_\pi) - s A(m_K) - \frac{m_\pi^2}{3} A(m_\eta) + \left(\frac{7}{3} m_\pi^2 - 2s\right) \log\left(\frac{m_\pi^2}{\mu^2}\right) + \left(\frac{2}{3} m_K^2 - s\right) \log\left(\frac{m_K^2}{\mu^2}\right) \\ &\quad - \frac{m_\eta^2}{3} \log\left(\frac{m_\eta^2}{\mu^2}\right) + \left(3s - \frac{2}{3} m_\pi^2\right). \end{aligned} \quad (\text{A.3})$$

In the above expressions μ is the renormalization scale, $s = (p_{\pi^-} + p_{\pi^+})^2$ is the square of the two-pion center of mass energy and

$$A(m) \equiv \sqrt{1 - 4\frac{m^2}{s}} \left(\log\left(\frac{1 + \sqrt{1 - 4m^2/s}}{1 - \sqrt{1 - 4m^2/s}}\right) - i\pi\theta\left(1 - 4\frac{m^2}{s}\right) \right). \quad (\text{A.4})$$

To the one-loop corrections listed in the above equations, we should add those proportional to the Gasser–Leutwyler coefficients, L_i [13], appearing at NLO in the strong interaction chiral Lagrangian. These effects, combined with I_z , are reabsorbed into the renormalization of the decay constant, leading to the replacement of the factor $1/f^2$ by $1/f_\pi^2$ in the matrix elements of the scalar operator. Since these terms do not affect the finite volume corrections which are the object of the present study, we will not discuss them further here. Similarly the matrix elements of the (higher-dimensional) counter-terms of the scalar density do not contribute to the finite volume effects and will not be considered.

The s -wave phase shift for the $I = 0$ two-pion state at one-loop in χ PT is given by

$$\delta(s) = \frac{2s - m_\pi^2}{16\pi f^2} \sqrt{1 - 4\frac{m_\pi^2}{s}}. \quad (\text{A.5})$$

For $s \geq 4m_\pi^2$, we have $\text{Arg}[\langle \pi^-(\vec{q}) \pi^+(-\vec{q}) | S | 0 \rangle] = \delta(s)$. Note that the amplitude remains finite at threshold, i.e., as $s \rightarrow 4m_\pi^2$.

Appendix B. The scalar amplitude in quenched QCD

In this appendix we discuss the matrix element of the scalar density in quenched QCD. The quenched chiral Lagrangian used in our calculations is:

$$\begin{aligned} \mathcal{L}_{\text{strong}}^q = & \left(\frac{f^2}{8} + \frac{v_1}{2} \Phi_0^2 \right) \text{str}[(\partial_\mu \Sigma^{q\dagger})(\partial^\mu \Sigma^q)] + \left(\frac{f^2}{8} + \frac{v_2}{2} \Phi_0^2 \right) \text{str}[\Sigma^{q\dagger} \chi + \chi^\dagger \Sigma^q] \\ & - m_0^2 \Phi_0^2 + \alpha (\partial_\mu \Phi_0)(\partial^\mu \Phi_0), \end{aligned} \quad (\text{B.1})$$

with the super- η' field, $\Phi_0 = f/2i \text{str}[\log \Sigma^q]/\sqrt{6}$.

The one-loop matrix element of the scalar operator in the quenched theory, at infinite volume, is given by

$$\langle \pi^+ \pi^- | S^q | 0 \rangle \equiv -\frac{8}{f^2} [1 + \mathcal{A}_\infty^q] = -\frac{8}{f^2} \left[1 + \frac{1}{(4\pi f)^2} (I_z^q + I_a^q + I_b^q) \right], \quad (\text{B.2})$$

where

$$\begin{aligned} I_z^q &= 0, \\ I_a^q &= -\frac{2m_\pi^2}{3} \log\left(\frac{m_\pi^2}{\mu^2}\right) - \frac{m_K^2}{3} \log\left(\frac{m_K^2}{\mu^2}\right) - \frac{2m_0^2}{3} \left[1 + \log\left(\frac{m_\pi^2}{\mu^2}\right) \right] + \frac{2}{3} \alpha m_\pi^2 \left[1 + 2 \log\left(\frac{m_\pi^2}{\mu^2}\right) \right], \\ I_b^q &= s \left(\frac{3}{2} - A(m_\pi) - \frac{1}{2} A(m_K) \right) + \left(\frac{2}{3} m_\pi^2 - s \right) \log\left(\frac{m_\pi^2}{\mu^2}\right) + \left(\frac{1}{3} m_K^2 - \frac{s}{2} \right) \log\left(\frac{m_K^2}{\mu^2}\right) \\ &+ \frac{2m_\pi^2(v_2 - v_1) + s v_1}{3} \left(A(m_{\bar{s}s}) + 2A(m_\pi) + 2 \log\left(\frac{m_\pi^2}{\mu^2}\right) + \log\left(\frac{m_{\bar{s}s}^2}{\mu^2}\right) - 3 \right) \\ &+ m_0^2 \left[\frac{4m_\pi^2}{3(s - 4m_\pi^2)} A(m_\pi) \right] + \alpha \frac{4m_\pi^2}{3} \left[\log\left(\frac{m_\pi^2}{\mu^2}\right) - 1 + \frac{s - 5m_\pi^2}{s - 4m_\pi^2} A(m_\pi) \right] \\ &+ m_0^4 \left[\frac{m_\pi^2}{18(m_K^2 - m_\pi^2)^2} (A_{10} - A(m_{\bar{s}s})) - \frac{8m_\pi^2}{9s(s - 4m_\pi^2)} + \frac{m_\pi^2}{9s(m_K^2 - m_\pi^2)} \log\left(\frac{m_{\bar{s}s}^2}{m_\pi^2}\right) \right. \\ &\quad \left. - \frac{m_\pi^2 [32m_\pi^6 + 16m_K^4(2m_\pi^2 - s) - 8m_\pi^2 s^2 + s^3 - 32m_K^2 m_\pi^2 (2m_\pi^2 - s)]}{18s(m_K^2 - m_\pi^2)^2 (s - 4m_\pi^2)^2} A(m_\pi) \right] \\ &+ \alpha m_0^2 \left[\frac{16m_\pi^4}{9s(s - 4m_\pi^2)} + \frac{m_\pi^2}{9(m_K^2 - m_\pi^2)^2} (m_{\bar{s}s}^2 A(m_{\bar{s}s}) - m_K^2 A_{10}) - \frac{m_\pi^2 (2m_K^2 - s)}{9s(m_K^2 - m_\pi^2)} \log\left(\frac{m_{\bar{s}s}^2}{m_\pi^2}\right) \right. \\ &\quad \left. + \frac{m_\pi^2 [8(m_K^2 - m_\pi^2)^2 (4m_\pi^4 + 2m_\pi^2 s - s^2) + m_\pi^2 s (s - 4m_\pi^2)^2]}{9s(m_K^2 - m_\pi^2)^2 (s - 4m_\pi^2)^2} A(m_\pi) \right] \\ &+ \frac{2m_\pi^2}{3} \alpha^2 \left[1 - \frac{4m_\pi^4}{3s(s - 4m_\pi^2)} + \frac{m_{\bar{s}s}^2}{12(m_K^2 - m_\pi^2)^2} (m_\pi^2 A_{10} - m_{\bar{s}s}^2 A(m_{\bar{s}s})) \right. \\ &\quad \left. - \frac{[8(m_K^2 - m_\pi^2)^2 (4m_\pi^6 + 22m_\pi^4 s - 10m_\pi^2 s^2 + s^3) + m_\pi^4 s (s - 4m_\pi^2)^2]}{12s(m_K^2 - m_\pi^2)^2 (s - 4m_\pi^2)^2} A(m_\pi) \right. \\ &\quad \left. - \frac{m_\pi^2 m_{\bar{s}s}^2 + s(4m_K^2 - 5m_\pi^2)}{6s(m_K^2 - m_\pi^2)} \log\left(\frac{m_\pi^2}{\mu^2}\right) - \frac{m_{\bar{s}s}^2 (s - m_\pi^2)}{6s(m_K^2 - m_\pi^2)} \log\left(\frac{m_{\bar{s}s}^2}{\mu^2}\right) \right], \end{aligned}$$

with

$$m_{\bar{s}s}^2 = 2m_K^2 - m_\pi^2,$$

$$A_{10} = \Lambda \log \left(\frac{1 - 2\frac{m_K^2}{s} + \Lambda}{1 - 2\frac{m_K^2}{s} - \Lambda} \right) - i\pi\theta(\sqrt{s} - (m_{\bar{s}s} + m_\pi)),$$

$$\Lambda = \sqrt{1 + 4\frac{m_K^4}{s^2} + 4\frac{m_\pi^4}{s^2} - 4\frac{m_K^2}{s} \left(1 + 2\frac{m_\pi^2}{s}\right)}.$$

The imaginary part of the amplitude diverges at threshold, i.e., as $s \rightarrow 4m_\pi^2$ [14,15].

Appendix C. Finite-volume scalar correlation function in full QCD

In this appendix we give the complete one-loop expression of the finite-volume correlation function of the scalar operator with two pion fields in the full theory:

$$\langle 0 | \pi_{-\bar{q}}^+(t_1) \pi_{\bar{q}}^-(t_2) S(0) | 0 \rangle = \frac{e^{-Et_1}}{2E} \frac{e^{-Et_2}}{2E} \left(-\frac{8}{f^2} \right) \left[1 + \frac{1}{(4\pi f)^2} (I_z + I_a) + I_b(t_1, t_2) \right], \quad (\text{C.1})$$

where $E = \sqrt{\vec{q}^2 + m_\pi^2}$. Since we are interested in finite volume corrections we give only the explicit expression for $I_b(t_1, t_2)$. We write

$$I_b(t_1, t_2) = -\frac{E^2}{2f^2} [A_{00} + A_{11} + A_{22}], \quad (\text{C.2})$$

where

$$\begin{aligned} A_{00} &= \frac{m_\pi^2}{6E^2} \frac{1}{L^3} \sum_{\vec{k}} \frac{1}{w_0^2} \left\{ \frac{1}{2(E-w_0)} - \frac{1}{2(E+w_0)} - e^{2(E-w_0)t_2} \left(\frac{1}{2(E-w_0)} + \frac{1}{2w_0} \right) \right. \\ &\quad \left. + e^{2Et_2-2w_0t_1} \left(\frac{1}{2w_0} - \frac{1}{2(w_0+E)} \right) \right\}, \\ A_{11} &= \frac{1}{L^3} \sum_{\vec{k}} \left\{ \frac{d_+(w_1)}{2(E-w_1)} - \frac{d_-(w_1)}{2(E+w_1)} - e^{2(E-w_1)t_2} \left(\frac{d_+(w_1)}{2(E-w_1)} + \frac{d_0(w_1)}{2w_1} \right) \right. \\ &\quad \left. + e^{2Et_2-2w_1t_1} \left(\frac{d_0(w_1)}{2w_1} - \frac{d_-(w_1)}{2(w_1+E)} \right) \right\}, \\ A_{22} &= \frac{1}{L^3} \sum_{\vec{k}} \left\{ \frac{c_+(w_2)}{2(E-w_2)} - \frac{c_-(w_2)}{2(E+w_2)} - e^{2(E-w_2)t_2} \left(\frac{c_+(w_2)}{2(E-w_2)} + \frac{c_0(w_2)}{2w_2} \right) \right. \\ &\quad \left. + e^{2Et_2-2w_2t_1} \left(\frac{c_0(w_2)}{2w_2} - \frac{c_-(w_2)}{2(w_2+E)} \right) \right\}. \end{aligned}$$

In the above expressions

$$\begin{aligned} w_0 &= \sqrt{\vec{k}^2 + m_{\bar{s}s}^2}, & w_1 &= \sqrt{\vec{k}^2 + m_\pi^2}, & w_2 &= \sqrt{\vec{k}^2 + m_K^2}, \\ c_\pm(w) &= \frac{2}{3} \frac{E^2 \pm Ew + w^2}{E^2 w^2}, & c_0(w) &= \frac{2}{3} \frac{1}{E^2}, & d_{\pm,0}(w) &= 2c_{\pm,0}(w) - \frac{m_\pi^2}{2E^2 w^2}. \end{aligned}$$

Evaluating the sums, we find

$$\langle 0 | \pi_{-\bar{q}}^+(t_1) \pi_{\bar{q}}^-(t_2) S(0) | 0 \rangle = \frac{e^{-Et_1}}{2E} \frac{e^{-Et_2}}{2E} \left(-\frac{8}{f^2} \right) [1 + \text{Re}(\mathcal{A}_\infty) + \mathcal{T}(t_2)], \quad (\text{C.3})$$

where, for $E < m_K < m_{\bar{s}s}$,

$$\begin{aligned} \mathcal{T}(t_2) = & -\frac{E^2}{2f^2} \left[-\frac{\nu t_2}{E^2 L^3} \left(4 - \frac{m_\pi^2}{2E^2} \right) + \left(2 - \frac{3m_\pi^2}{4E^2} \right) \left(-\frac{\nu}{3E^3 L^3}; -\frac{\nu}{6E^3 L^3} \right) \right. \\ & \left. + \left(\frac{z(0)}{E^3 L^3} \left(1 - \frac{3m_\pi^2}{8E^2} \right) - \frac{z(1)}{\pi^2 EL} \left(1 - \frac{m_\pi^2}{8E^2} \right) \right) \right] \end{aligned} \quad (\text{C.4})$$

and $\nu = \sum_{\vec{k}:w=E} \bar{q}$. We have used

$$z(s) = \sum_{|\vec{l}| \neq |\vec{n}|} \frac{1}{(\vec{l}^2 - \vec{n}^2)^s} \quad \text{and} \quad \bar{q} = \frac{2\pi}{L} \vec{n}. \quad (\text{C.5})$$

When we take the large-volume limit at fixed two-pion energy, W , we expect that $z(s)$ scales as $L^{(2-2s)}$ (and that $z(0) \sim -\nu \sim L^2$). Thus the finite volume corrections decrease as $1/L$ when $L \rightarrow \infty$ [16].

The terms $(\dots; \dots)$ are the forward time contributions (FTCs) for the two cases $t_1 \gg t_2$ and $t_2 = t_1$, respectively. These are the terms which are reabsorbed by the sink when the matrix element is extracted (for a detailed discussion see Section 4.1 of Ref. [4]).

From the above equations we find

$$\begin{aligned} \Delta W = & -\frac{\nu}{4f^2 L^3} \left(8 - \frac{m_\pi^2}{E^2} \right) \rightarrow -\frac{7}{4f^2 L^3} \implies a_0 = \frac{7m_\pi}{16\pi f^2}, \\ \sqrt{LL} = & 1 - \frac{E^2}{2f^2} \left[\frac{\nu}{(EL)^3} \left(\frac{3m_\pi^2}{8E^2} - 1 \right) - \frac{z(1)}{\pi^2 EL} \left(1 - \frac{m_\pi^2}{8E^2} \right) \right] \rightarrow 1 + \frac{m_\pi^2}{16\pi^2 f^2} \left(\frac{7z(1)}{m_\pi L} + \frac{5\pi^2}{(m_\pi L)^3} \right), \\ \text{FTCs} = & 1 + \left(1 - \frac{3m_\pi^2}{8E^2} \right) \left(\frac{\nu}{3f^2 EL^3}; \frac{\nu}{6f^2 EL^3} \right) \rightarrow 1 + \left(\frac{5}{24f^2 m_\pi L^3}; \frac{5}{48f^2 m_\pi L^3} \right), \end{aligned} \quad (\text{C.6})$$

where the limits refer to the case with the two pions at rest. All these results are in agreement with expectations: the energy shift in a finite volume is precisely the one predicted by the Lüscher quantization condition [6]; the LL factor is in agreement with the general formula of Ref. [1] and the FTCs term will be cancelled when we divide the correlation function by the square root of the $\pi\pi \rightarrow \pi\pi$ correlator of Eq. (7).

Appendix D. Finite-volume scalar correlation function in quenched QCD

In this appendix we give the complete one-loop expression of the finite-volume correlation function for the scalar operator with two pion fields in the quenched theory:

$$\langle 0 | \pi_{-\vec{q}}^+(t_1) \pi_{\vec{q}}^-(t_2) S^q(0) | 0 \rangle = \frac{e^{-Et_1}}{2E} \frac{e^{-Et_2}}{2E} \left(-\frac{8}{f^2} \right) \left[1 + \frac{1}{(4\pi f)^2} (I_z^q + I_a^q) + I_b^q(t_1, t_2) \right], \quad (\text{D.1})$$

where

$$I_b^q(t_1, t_2) = -\frac{E^2}{2f^2} [A_{00} + A_{10} + A_{11} + A_{22}], \quad (\text{D.2})$$

with

$$\begin{aligned}
A_{00} &= a_{00} \frac{1}{L^3} \sum_{\vec{k}} \frac{1}{w_0^2} \left\{ \frac{1}{2(E-w_0)} - \frac{1}{2(E+w_0)} - e^{2(E-w_0)t_2} \left(\frac{1}{2(E-w_0)} + \frac{1}{2w_0} \right) \right. \\
&\quad \left. + e^{2Et_2-2w_0t_1} \left(\frac{1}{2w_0} - \frac{1}{2(w_0+E)} \right) \right\} \\
&\quad + \frac{1}{L^3} \sum_{\vec{k}} \frac{1}{w_0^2} \left\{ \frac{b}{2(E-w_0)} - \frac{b}{2(E+w_0)} - e^{2(E-w_0)t_2} \left(\frac{b}{2(E-w_0)} + \frac{\tilde{b}}{2w_0} \right) \right. \\
&\quad \left. + e^{2Et_2-2w_0t_1} \left(\frac{\tilde{b}}{2w_0} - \frac{b}{2(w_0+E)} \right) \right\}, \\
A_{10} &= a_{10} \frac{1}{L^3} \sum_{\vec{k}} \frac{1}{w_0 w_1} \left\{ \frac{1}{2E-w_0-w_1} - \frac{1}{2E+w_0+w_1} - e^{(2E-w_0-w_1)t_2} \left(\frac{1}{2E-w_0-w_1} + \frac{1}{w_0+w_1} \right) \right. \\
&\quad \left. + e^{2Et_2-(w_0+w_1)t_1} \left(\frac{1}{w_0+w_1} - \frac{1}{w_0+w_1+2E} \right) \right\}, \\
A_{11} &= \frac{1}{L^3} \sum_{\vec{k}} \left\{ \frac{c_+(w_1)}{2(E-w_1)} - \frac{c_-(w_1)}{2(E+w_1)} - e^{2(E-w_1)t_2} \left(\frac{c_+(w_1)}{2(E-w_1)} + \frac{c_0(w_1)}{2w_1} \right) \right. \\
&\quad \left. + e^{2Et_2-2w_1t_1} \left(\frac{c_0(w_1)}{2w_1} - \frac{c_-(w_1)}{2(w_1+E)} \right) \right\} \\
&\quad + \frac{2}{L^3} \sum_{\vec{k}} \frac{1}{w_1^2} \left\{ \frac{b}{2(E-w_1)} - \frac{b}{2(E+w_1)} - e^{2(E-w_1)t_2} \left(\frac{b}{2(E-w_1)} + \frac{\tilde{b}}{2w_1} \right) \right. \\
&\quad \left. + e^{2Et_2-2w_1t_1} \left(\frac{\tilde{b}}{2w_1} - \frac{b}{2(w_1+E)} \right) \right\} \\
&\quad + \frac{1}{L^3} \sum_{\vec{k}} \frac{a_{11}^{(1)}(w)}{E^2} \left\{ \frac{1}{2(E-w_1)} - \frac{1}{2(E+w_1)} - e^{2(E-w_1)t_2} \left(\frac{1}{2(E-w_1)} + \frac{1}{2w_1} \right) \right. \\
&\quad \left. + e^{2Et_2-2w_1t_1} \left(\frac{1}{2w_1} - \frac{1}{2(w_1+E)} \right) \right\} \\
&\quad + \frac{1}{L^3} \sum_{\vec{k}} \frac{a_{11}^{(2)}(w)}{E} \left\{ \frac{1}{[2(E-w_1)]^2} + \frac{1}{[2(E+w_1)]^2} - e^{2(E-w_1)t_2} \left(\frac{1-[2(E-w_1)]t_2}{[2(E-w_1)]^2} - \frac{1+[2w_1]t_2}{[2w_1]^2} \right) \right. \\
&\quad \left. - e^{2Et_2-2w_1t_1} \left(\frac{1+[2w_1]t_1}{[2w_1]^2} - \frac{1+[2(w_1+E)]t_1}{[2(w_1+E)]^2} \right) \right\} \\
&\quad + \frac{1}{L^3} \sum_{\vec{k}} a_{11}^{(3)}(w) \left\{ \frac{1}{[2(E-w_1)]^3} - \frac{1}{[2(E+w_1)]^3} \right. \\
&\quad \left. - e^{2(E-w_1)t_2} \left(\frac{1-[2(E-w_1)]t_2 + [2(E-w_1)]^2 t_2^2 / 2}{[2(E-w_1)]^3} + \frac{1+[2w_1]t_2 + [2w_1]^2 t_2^2 / 2}{[2w_1]^3} \right) \right. \\
&\quad \left. + e^{2Et_2-2w_1t_1} \left(\frac{1+[2w_1]t_1 + [2w_1]^2 t_1^2 / 2}{[2w_1]^3} - \frac{1+[2(w_1+E)]t_1 + [2(w_1+E)]^2 t_1^2 / 2}{[2(w_1+E)]^3} \right) \right\},
\end{aligned}$$

$$A_{22} = \frac{1}{2L^3} \sum_{\vec{k}} \left\{ \frac{c_+(w_2)}{2(E-w_2)} - \frac{c_-(w_2)}{2(E+w_2)} - e^{2(E-w_2)t_2} \left(\frac{c_+(w_2)}{2(E-w_2)} + \frac{c_0(w_2)}{2w_2} \right) \right. \\ \left. + e^{2Et_2-2w_2t_1} \left(\frac{c_0(w_2)}{2w_2} - \frac{c_-(w_2)}{2(w_2+E)} \right) \right\}.$$

In the above equations

$$b = \tilde{b} - \frac{2}{3}v_1, \quad \tilde{b} = \frac{m_\pi^2(v_1 - v_2)}{3E^2}, \\ a_{00} = \frac{y[m_0^2 - \alpha m_K^2(2-y)]^2}{36E^2 m_K^2(1-y)^2}, \quad a_{10} = -\frac{y[m_0^2 - \alpha m_K^2 y][m_0^2 - \alpha m_K^2(2-y)]}{18E^2 m_K^2(1-y)^2}, \\ a_{11}^{(1)}(w_1) = -\frac{m_0^2 m_K^2 y}{3w_1^4} + \frac{\alpha m_K^2 y (ym_K^2 - 2w_1^2)}{3w_1^4} \\ + \frac{m_0^4 y [w_1^4 + 2m_K^4(1-y)^2] - 2\alpha m_0^2 y m_K^2 [(1-y)^2(-4m_K^2 w_1^2 + 2m_K^4 y) + yw_1^4]}{36m_K^2 w_1^6(1-y)^2} \\ + \frac{\alpha^2 m_K^4 y [2m_K^2 y(1-y)^2(-4w_1^2 + ym_K^2) + w_1^4(8 - 16y + 9y^2)]}{36m_K^2 w_1^6(1-y)^2}, \\ a_{11}^{(2)}(w_1) = -\frac{ym_K^2 [m_0^2 - \alpha m_K^2 y][m_0^2 - \alpha m_K^2 y + (2\alpha - 3)w_1^2]}{9Ew_1^5}, \\ a_{11}^{(3)}(w_1) = \frac{ym_K^2 [m_0^2 - \alpha m_K^2 y]^2}{9E^2 w_1^4}.$$

m_0 and α are the parameters characterizing the η' propagator [4]. Evaluating the sums, we obtain:

$$\langle 0 | \pi_{-\vec{q}}^+(t_1) \pi_{\vec{q}}^-(t_2) S^q(0) | 0 \rangle = \frac{e^{-Et_1}}{2E} \frac{e^{-Et_2}}{2E} \left(-\frac{8}{f^2} \right) [1 + \text{Re}(A_\infty^q) + T^q(t_2)], \quad (\text{D.3})$$

where, for $E \leq m_K \leq m_{\bar{s}s}$ we have

$$T^q(t_2) = -\frac{E^2}{2f^2} \left[-\frac{2vt_2}{E^2 L^3} + \left(-\frac{v}{3E^3 L^3}; -\frac{v}{6E^3 L^3} \right) + \left(\frac{z(0)}{2E^3 L^3} - \frac{z(1)}{2\pi^2 EL} \right) \right] \\ + \left[-\frac{2bvt_2}{E^2 L^3} + \left(-\frac{v\tilde{b}}{E^3 L^3}; -\frac{vb}{2E^3 L^3} \right) + \left(\frac{3bz(0)}{2E^3 L^3} - \frac{bz(1)}{2\pi^2 EL} \right) \right] \\ + a_{11}^{(1)}(E) \left[-\frac{vt_2}{E^2 L^3} + \left(-\frac{v}{2E^3 L^3}; -\frac{v}{4E^3 L^3} \right) + \left(\frac{b_{11}^{(1)}(E)}{a_{11}^{(1)}(E)} \frac{z(0)}{4E^3 L^3} - \frac{z(1)}{4\pi^2 EL} \right) \right] \\ + a_{11}^{(2)}(E) \left[\frac{vt_2^2/2}{EL^3} + \left(\frac{(1+2Et_2)v}{4E^3 L^3}; \frac{(1+4Et)v}{16E^3 L^3} \right) + \left(\frac{c_{11}^{(2)}(E)z(0)}{16E^3 L^3} + \frac{b_{11}^{(2)}(E)z(1)}{4\pi^2 EL} + \frac{z(2)}{16\pi^4 EL} \right) \right] \\ + a_{11}^{(3)}(E) \left[\frac{vt_2^3/6}{L^3} + \left(-\frac{(1+2Et_2+2E^2t_2^2)v}{8E^3 L^3}; -\frac{(1+4Et+8E^2t^2)v}{64E^3 L^3} \right) \right. \\ \left. + \left(\frac{111z(0)}{64E^3 L^3} - \frac{3z(1)}{8\pi^2 EL} + \frac{5z(2)}{64\pi^4 EL} - \frac{z(3)}{64\pi^6 (EL)^3} \right) \right], \quad (\text{D.4})$$

$$\begin{aligned}
b_{11}^{(1)}(E) &= -\frac{7m_0^2 m_K^2 y}{3E^4} + \frac{\alpha m_K^2 y (7ym_K^2 - 6E^2)}{3E^4} \\
&+ \frac{m_0^4 y [3E^4 + 22m_K^4 (1-y)^2] - 2\alpha m_0^2 y m_K^2 [(1-y)^2 (-28m_K^2 E^2 + 22m_K^4 y) + 3yE^4]}{36m_K^2 E^6 (1-y)^2} \\
&+ \frac{\alpha^2 m_K^4 y [2m_K^2 y (1-y)^2 (-28E^2 + 11ym_K^2) + 3E^4 (8 - 16y + 9y^2)]}{36m_K^2 E^6 (1-y)^2}, \\
c_{11}^{(2)}(E) &= \frac{17E^2(2\alpha - 3) + 49m_0^2 - 49y\alpha m_K^2}{E^2(2\alpha - 3) + m_0^2 - y\alpha m_K^2}, \\
b_{11}^{(2)}(E) &= -\frac{E^2(2\alpha - 3) + 2m_0^2 - 2y\alpha m_K^2}{E^2(2\alpha - 3) + m_0^2 - y\alpha m_K^2}.
\end{aligned}$$

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