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Multiple-channel generalization of Lellouch-Lüscher formula

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We generalize the Lellouch-Lüscher formula, relating weak matrix elements in finite and infinite volumes, to the case of multiple strongly-coupled decay channels into two scalar particles. This is a necessary first step on the way to a lattice QCD calculation of weak decay rates for processes such as $D \rightarrow \pi\pi$ and $D \rightarrow K\bar{K}$. We also present a field theoretic derivation of the generalization of Lüscher's finite volume quantization condition to multiple two-particle channels. We give fully explicit results for the case of two channels, including a form of the generalized Lellouch-Lüscher formula expressed in terms of derivatives of the energies of finite volume states with respect to the box size. Our results hold for arbitrary total momentum and for degenerate or non-degenerate particles.

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I. INTRODUCTION

Lattice calculations have made considerable progress toward a first-principles determination of the $K \rightarrow \pi\pi$ weak decay amplitudes [1, 2]. The methodology is now in place, results for the $I = 2$ final state with a complete error budget are available [2], and complete results for the more challenging $I = 0$ final states should become available in the next few years. At that stage we will finally learn whether and in what manner QCD can explain the $\Delta I = 1/2$ rule and the observed CP-violation rate in $K \rightarrow \pi\pi$ decays.

Encouraged by this progress, it is natural to consider what information lattice calculations might eventually offer concerning the decays of heavier mesons. For example, the LHCb experiment recently reported evidence for CP-violation in (the difference of) $D^0 \rightarrow \pi^+\pi^-$ and $D^0 \rightarrow K^+K^-$ decays [3]. Although the rate is larger than naive expectations from the Standard Model (SM), there is, at present, sufficient uncertainty in the SM prediction for it to be consistent with the LHCb result (see, e.g. Refs. [4–9]). This raises the obvious question of whether a calculation using lattice methods is feasible.

The aim of this paper is to take a first step in developing the methodology for such a calculation. We show how, if one can ignore all but two-particle channels, then a generalization of the work of Lüscher, and of Lellouch and Lüscher, would allow, in principle, a calculation of the required matrix elements from lattice calculations in a finite volume. In practice, however, channels with more than two particles are coupled by the strong interactions to $\pi\pi$ and $K\bar{K}$, e.g. the four pion channel, and they cannot be ignored at center of mass (CM) energies as high as the D^0 -meson mass ($M_{D^0} = 1865$ MeV). Thus our method would yield only semi-quantitative results for the desired matrix elements. Nevertheless, it

is a necessary first step, and work is underway to extend the methodology to channels with multiple particles (see, e.g., Ref. [10]).

It is instructive to recall the three essential ingredients needed for the lattice calculation of $K \rightarrow \pi\pi$ amplitudes. First, one needs to know the relation between the energies of two-pion states in a finite box and the infinite-volume scattering amplitude. This was worked out by Lüscher in Refs. [11–14] (and generalized to a moving frame in Refs. [15–17]). Second, one needs the relation between the matrix element that one can determine on the lattice, which connects a kaon to a finite-volume two pion state, and the infinite volume matrix element which determines the decay rate. This was provided by Lellouch and Lüscher in Ref. [18] (and generalized to a moving frame in Refs. [16, 17]). Finally, one must calculate the large number of Wick contractions that contribute, including several quark-disconnected contractions requiring special methods and high statistics. In this stage one also extrapolates to physical quark masses. This entire program has been carried out for the $I = 2$ final state [2], and a successful pilot calculation has been done for the more challenging $I = 0$ case [1].

The calculation of D^0 decays is considerably more challenging. In particular, the first two of the three aforementioned ingredients need to be generalized to account for the opening of many channels. If we focus on the $I = 0$ final state, then strong-interaction rescattering connects two-pion final states to those with four, six, etc. pions, as well as $K\bar{K}$ and $\eta\eta$ states.¹ As already noted, we consider here only the case in which several two-particle channels are open, which for the D^0 would mean keeping the $\pi\pi$, $K\bar{K}$ and $\eta\eta$ channels while ignoring those with

¹ It is important to note that the fact that the D^0 has a very large number of decay channels [19] is not itself a concern, but rather that, having fixed the final-state quantum numbers, in our case to $I = 0$, there are still a large number of states. In a lattice calculation, one can separately consider the decays to states with differing strong-interaction quantum numbers.

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four or more pions. We make this approximation not because we think that it is a good description of reality at the D^0 mass, but rather because it is a necessary first step towards the required formalism.

Within this approximation, we provide here the generalization of both the Lüscher quantization condition and the Lellouch-Lüscher (LL) formula. These generalizations are useful also in many other systems. For example, the quantization condition allows the determination of the parameters of the S -matrix in the $I = 0$ channel above the two kaon threshold (and thus in the region of the $f_0(980)$ resonance), because the coupling to four or more pions remains weak for such energies. The same should be true in the $I = 1$ case, where $K\bar{K}$ and $\eta\pi$ are the dominant channels in the vicinity of the $a_0(980)$. The multi-channel LL formula can be used to calculate $K \rightarrow \pi\pi$ amplitudes including isospin breaking (so that π^\pm and π^0 are not degenerate). Generalization to baryon decays are also possible, but this requires dealing with particles with spin, which we do not attempt here.

There have been a large number of recent papers studying the generalization of the Lüscher quantization condition to multiple two-body channels [20–23] and assessing its utility. The work of Ref. [20] uses non-relativistic quantum mechanics, while Ref. [21] is based on a non-relativistic effective field theory. References [22] and [23] are based on relativistic field theory, and give an explicit result [Eq. (3.5) of Ref. [22]] for the case of two s-wave channels in which the total momentum vanishes and in which the contributions from higher partial waves are assumed negligible. We also note that the multiple channel problem has been studied using an alternative approach based on the Bethe-Salpeter wavefunction [24].

We provide here, as a step on the way to the generalized LL formula, a derivation of the multiple-channel quantization condition within quantum field theory. We include all allowed mixing between different partial waves. No assumptions about the form of the interactions are needed, aside from the proviso, common to all approaches, that the range of the interaction must be smaller than the box size. Also, our result holds for any value of the total momentum \vec{P} of the two particle system (i.e. it holds for a moving or a stationary frame), and for either degenerate or non-degenerate particles in each channel. We follow closely the approach of Ref. [16], which presented a generalization of Lüscher's single-channel quantization condition to a moving frame. Indeed, we find that the most general form of the final result, given in Eq. (29), is identical in form to that of Ref. [16] (modulo some minor changes in notation).

After deriving the general quantization condition in Sec. II we restrict our considerations to the simplified situation in which only s-wave scattering is included. We focus on the case with two channels (suggestively labeled $\pi\pi$ and $K\bar{K}$), although we also provide the generalization to more than two channels. In the infinite volume theory, the two-channel system is described by a 2×2 S -matrix which, due to unitarity and symmetry, is de-

termined by three real parameters [see Eq.(48) below]. We use a particular parametrization of S to rewrite our quantization condition in a convenient, pure real form [Eq. (49)]. We explain how our result is equivalent to that of Ref. [22] in the case of a stationary frame. As is discussed in Refs. [21–23], three independent pieces of information are needed to determine the three independent S -matrix parameters at each center of mass energy, E^* . References [22] and [23] discuss in some detail the prospects for using either twisted boundary conditions or uneven box sizes for this purpose. We restrict ourselves here to an alternative approach, also mentioned in Refs. [22] and [23], of using three different choices for the parameters $\{L, \vec{P}\}$, where L is the box size. (We assume a cubic box and periodic boundary conditions.) The parameters $\{L, \vec{P}\}$ must be tuned such that there is a two-particle state in the spectrum having the desired value of E^* . In this way one obtains three independent conditions, and can solve for the S -matrix parameters at the chosen value of E^* .

Turning now to the LL formula, we follow the same approach as used by Lellouch and Lüscher in Ref. [18]. Specifically, we add a D -meson to our two-channel system and analyze the effect of an infinitesimal weak perturbation on the quantization condition. This yields a relation between a finite-volume weak matrix element and a linear combination of the desired infinite-volume matrix elements. In Sec. IV we present a derivation of the relation which follows closely the original LL work. In the final result, Eq. (85), the coefficients relating finite and infinite volume matrix elements are given in terms of the S -matrix parameters and their derivatives, evaluated at the decay particle's mass. These can be calculated using the multiple-channel quantization condition, as sketched above. It turns out that three different lattice matrix elements are needed to separately determine the two infinite-volume matrix elements. Note that this is the same as the number needed to determine the S -matrix parameters. For more than two channels this correspondence no longer holds.

Since the S -matrix parameters and their derivatives are ultimately determined from the spectral energies, it should be possible to write a form for the generalized LL formula in terms of the spectral energies and their derivatives alone. We derive such a form in Sec. V. The result, Eq. (122), is probably more useful in practice than Eq. (85). The second derivation also brings out an important feature of the generalized LL formula. Finite-volume energy eigenstates in the coupled-channel theory can be written as linear combinations of infinite volume $\pi\pi$ and $K\bar{K}$ states having (in our case) $\ell = 0$ as well as the higher values of ℓ allowed by the cubic symmetry of the box. The LL methodology is (as noted in the original paper) simply a trick to determine the coefficients of the relevant $\pi\pi$ and $K\bar{K}$ states. This point has also been stressed recently by Ref. [25] in a different context. Our second derivation makes clear that, irrespective of the details of the weak Hamiltonian, one always obtains

the same linear combination of $\pi\pi$ and $K\bar{K}$ states, and that this feature holds for any number of channels.

The remainder of this article is organized as follows. In the following section we give our derivation of the multiple channel quantization condition. In Sec. III we restrict to s -wave scattering and derive a useful form of the condition. The multiple channel generalization of the LL formula is then derived in Sec. IV, and the alternative derivation is presented in Sec. V. We conclude in Sec. VI. We include an appendix, in which we discuss the generalization of Watson's theorem to two channels.

The generalization of Lüscher's quantization formula to multiple channels for arbitrary \vec{P} using field-theoretic methods (the work described in our Secs. II and III) has also been considered by Briceno and Davoudi [26]. Our results are in complete agreement (although we use a different parametrization of the S -matrix). Their paper is being released simultaneously with the present article.

II. MULTIPLE CHANNEL EXTENSION OF QUANTIZATION CONDITION

In this section we derive an extension to multiple two-body channels of the Lüscher quantization condition, which relates the infinite volume scattering amplitudes to finite volume energy levels. We assume throughout a cubic spatial volume with extent L and periodic boundary conditions. The (Minkowski) time direction is taken to be infinite. The total momentum

$$\vec{P} = \frac{2\pi\vec{n}_P}{L} \quad (\vec{n}_P \in \mathbb{Z}^3) \quad (1)$$

is fixed but arbitrary, i.e. the quantization condition we derive holds for a “moving frame” as well as a stationary frame. We first consider the case of only two open channels, describing the extension to an arbitrary number of channels at the end of this section.

We take each channel to contain two massive, spinless particles. The particles of channel one are labeled pions and are taken to be identical with mass $m_1 = M_\pi$. The particles of channel two, called kaons, are taken non-identical, though still degenerate, with mass $m_2 = M_K$. What we have in mind is that the first channel corresponds to the $I = 0$ $\pi\pi$ state, and the second to the $I = 0$ $K\bar{K}$ state. Including both identical and non-identical pairs allows us to display the factors of 1/2 that appear in the former case. We consider degenerate particles to simplify the presentation, but describe the generalization to non-degenerate masses at the end of this section.

For concreteness, and to match the physical ordering, we take the pion to be lighter than the kaon. For our results to hold, we must assume that the thresholds for three or more particles lie above the two kaon threshold. If we assume a G-parity like symmetry, so that only even numbers of pions can couple to a two-pion state, then the ordering we need is

$$2M_\pi < 2M_K < E^* < 4M_\pi, \quad (2)$$

where E^* is the center of mass (CM) energy. The only possible scattering events are then

$$\begin{aligned} 1 \rightarrow 1: & \quad \pi\pi \rightarrow \pi\pi \\ 1 \rightarrow 2: & \quad \pi\pi \rightarrow K\bar{K} \\ 2 \rightarrow 1: & \quad K\bar{K} \rightarrow \pi\pi \\ 2 \rightarrow 2: & \quad K\bar{K} \rightarrow K\bar{K}. \end{aligned} \quad (3)$$

If E^* drops below $2M_K$, only the $\pi\pi$ channel is open and the problem reduces to that discussed by Lüscher [11–14].

The inequality $2M_K < 4M_\pi$ does not, of course, hold for physical pions and kaons—the four and six pion thresholds occur below that for two kaons. Nevertheless, the coupling to these higher multiplicity channels is weak at low energies, and our results should still hold approximately as long as we are not too far above the two kaon threshold. Indeed, it may be that, in the $I = 0$ case, the $\eta\eta$ channel becomes important before that with four or more pions. If so, our formalism would still apply, generalized to three channels as described below. The approximation of ignoring channels with more than two particles will become increasingly poor as the energy increases, and will likely give only a rough guide by the D mass. A qualitative indication of this (ignoring differences in phase space) is that the $f_0(1500)$ has a 50% branching fraction to 4π , while the branches to $\pi\pi$, $K\bar{K}$ and $\eta\eta$ are $\sim 35\%$, 9% and 5% , respectively [19].

The two channel quantization condition is obtained by a straightforward generalization of the single-channel approach of Ref. [16]. To make this note somewhat independent of that reference, we reiterate some of the pertinent details. We begin by introducing a two body interpolating field $\sigma(x)$ (not necessarily local) which couples to both channels. Following Ref. [16] we then define

$$C_L(P) = \int_{L;x} e^{i(-\vec{P}\cdot\vec{x} + Ex^0)} \langle 0 | \sigma(x) \sigma^\dagger(0) | 0 \rangle \quad (4)$$

where $P = (E, \vec{P})$ is the total four momentum of the two particle system (in the frame where the finite volume condition is applied), and

$$\int_{L;x} = \int_L d^4x \quad (5)$$

is the spacetime integral over finite volume. The relation to the CM energy used above is

$$E^* = \sqrt{E^2 - \vec{P}^2}. \quad (6)$$

The poles of C_L give the energy spectrum of the finite volume theory, and thus the condition that C_L diverge is precisely the quantization condition we are after.

To proceed to a more useful form of the condition, we follow Ref. [16] and write C_L in terms of the Bethe-

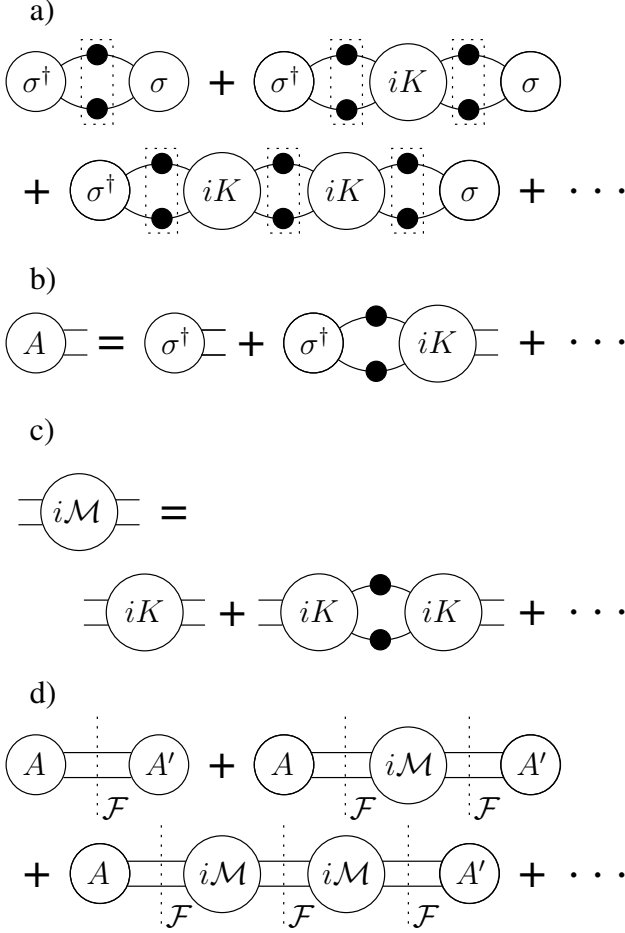


FIG. 1. (a) The initial series of ladder diagrams which builds up C_L [see Eq. (7)]. The Bethe-Salpeter kernels iK are connected by fully dressed propagators. The dashed rectangle indicates finite volume momentum sum/integrals. (b) and (c) The series which build up the matrix element A and the scattering amplitude iM . Note that these series contain only the momentum integrals appropriate to *infinite* volume. (d) The resulting series for the subtracted correlator [see Eqs. (17) and (26)]. Each dashed vertical line indicates an insertion of \mathcal{F} , which carries the entire volume dependence (neglecting exponentially suppressed dependence).

Salpeter kernel, as illustrated in Fig. 1(a):

$$C_L(P) = \int_{L;q} \sigma_{j,q} [z^2 \Delta^2]_{jk,q} \sigma_{k,q}^\dagger + \int_{L;q,q'} \sigma_{j,q} [z^2 \Delta^2]_{jk,q} iK_{kl;q,q'} [z^2 \Delta^2]_{lm,q'} \sigma_{m,q'}^\dagger + \dots \quad (7)$$

The notation here is as follows. Indices j , k , l and m refer to the channel, and take the values 1 or 2. The two particle intermediate states are summed/integrated as is

appropriate to finite volume

$$\int_{L,q} = \frac{1}{L^3} \sum_{\vec{q}} \int \frac{dq^0}{2\pi}. \quad (8)$$

The summand/integrand includes the product of two fully dressed propagators

$$[z^2 \Delta^2]_{ij,q} = \delta_{ij} \eta_i [z_i(q) \Delta_i(q)] [z_i(P-q) \Delta_i(P-q)], \quad (9)$$

where

$$z_j(q) \Delta_j(q) = \int d^4x e^{iqx} \langle \phi_j(x) \phi_j(0) \rangle \quad (10)$$

$$\Delta_j(q) = \frac{i}{q^2 - m_j^2 + i\epsilon}. \quad (11)$$

Here ϕ_1 and ϕ_2 are interpolating fields for pions and kaons, respectively, chosen such that $z_j = 1$ on shell. $\eta_1 = 1/2$ and $\eta_2 = 1$ account for the symmetry factors of the diagrams. K is related to the Bethe-Salpeter kernel

$$iK_{ij;q,q'} = iBS_{ij}(q, P-q, -q', -P+q'), \quad (12)$$

with BS_{ij} the sum of all amputated $j \rightarrow i$ scattering diagrams which are two-particle-irreducible in the s -channel (with particles of either type). Finally, $\sigma_{j,q}$ and $\sigma_{j,q'}^\dagger$ describe the coupling of the operators σ and σ^\dagger to the two-particle channel j . Their detailed form is not relevant; all we need to know is that they are regular functions of q .

We emphasize two important features of Eq. (7). First, it does not rely on any choice of interactions between the pions and kaons, such as those predicted by chiral perturbation theory. All the quantities that enter can be written in terms of non-perturbatively defined correlation functions. Second, the kernel iK and the propagator dressing function z have only exponentially suppressed dependence on the volume [12]. Thus, if L is large enough that such dependence is negligible (as we assume hereafter), we can take iK and z to have their infinite-volume forms.

The dominant power-law volume dependence enters through the momentum sums in the two-particle loops. To extract this dependence, we use the identity derived in Ref. [16], which relates these sums for a moving frame to infinite-volume momentum integrals plus a residue. Before stating the identity we recall the relevant notation. For any four vector $k^\mu = (k^0, \vec{k})$ in the moving frame, $k^{\mu*} = (k^{0*}, \vec{k}^*)$ is the result of a boost to the CM frame. In particular, the total four-momentum (E, \vec{P}) boosts to $(E^*, \vec{0})$ in the CM frame. We also need the quantities

$$q_j^* = \sqrt{(E^*)^2/4 - m_j^2}, \quad (13)$$

which are the momenta of a pion ($j = 1$) or kaon ($j = 2$) in the CM frame. The identity then reads (no sum on i

here):

$$\begin{aligned} \int_{L;k} f(k) \eta_i \Delta_i(k) \Delta_i(P-k) g(k) = \\ \int_{\infty;k} f(k) \eta_i \Delta_i(k) \Delta_i(P-k) g(k) \\ + \int d\Omega_{q^*} d\Omega_{q^{*\prime}} f_i^*(\hat{q}^*) \mathcal{F}_{ii}(\hat{q}^*, \hat{q}^{*\prime}) g_i^*(\hat{q}^{*\prime}), \end{aligned} \quad (14)$$

with

$$\int_{\infty;k} = \int \frac{d^4 k}{(2\pi)^4}. \quad (15)$$

We introduce two functions $f(k)$ and $g(k)$ to correspond to the momentum dependence entering from the left and right of the loop integrals, as well as that from the dressing functions [see Fig. 1(a)]. The functions f and g must have ultraviolet behavior that renders the integral/sum convergent. In addition, the branch cuts they contain, corresponding to four or more intermediate particles, must be such that, after the k^0 contour integration, they introduce no singularities for real \vec{k} . This condition holds when $0 < E^* < 4M_\pi$. The last line of (14) depends on the values of the functions f and g when the two particles are on-shell, and thus only on the direction of the CM momentum, \hat{q}^* . Specifically, if q_i^μ is the moving frame momentum that boosts to the on-shell momentum $(E^*/2, \vec{q}_i^*)$, then

$$f_i^*(\hat{q}^*) = f(q_i), \quad g_i^*(\hat{q}^*) = g(q_i). \quad (16)$$

Finally the quantity \mathcal{F} , which depends on q^* , L and the particle mass, contains the power-law finite-volume dependence of the loop sum/integral.² Its form is given below in Eqs. (23)-(25). Note that it is diagonal in channel space, i.e. it cannot change pions into kaons. It can, however, insert angular momentum, due to the breaking of rotation symmetry by the cubic box.

The key point of the identity is that the difference between finite and infinite volume integrals depends on *on-shell* values of the integrand, allowing the finite-volume dependence to be expressed in terms of physical quantities. Applying the identity to each loop integral in Fig. 1(a), one then rearranges the series by grouping terms with the same number of insertions of \mathcal{F} . The volume-independent term with no \mathcal{F} insertions is of no interest, since it does not lead to poles. Thus we drop it and consider the difference

$$C_{\text{sub}}(P) \equiv C_L(P) - C_\infty(P). \quad (17)$$

In the remaining diagrams with \mathcal{F} insertions, all terms to the left of the first \mathcal{F} and to the right of the last are grouped and summed into new endcaps which we label A_j and A'_j [see Fig. 1(b)]. These quantities equal certain matrix elements of the interpolating field σ [16]

$$A_j(\hat{k}^*) \equiv \langle \vec{k}^*, -\vec{k}^*; j; \text{out} | \sigma^\dagger(0) | 0 \rangle_{|\vec{k}^*|=q_j^*} \quad (18)$$

$$A'_j(\hat{k}^*) \equiv \langle 0 | \sigma(0) | \vec{k}^*, -\vec{k}^*; j; \text{in} \rangle_{|\vec{k}^*|=q_j^*}. \quad (19)$$

In contrast to [16] we include no wavefunction renormalization factors, because our single particle interpolating fields satisfy on-shell renormalization conditions. Having summed up the ends the next step is to do the same for the series which appears between adjacent \mathcal{F} insertions [Fig. 1(c)]. As indicated in the figure, this series generates the infinite volume scattering amplitude $i\mathcal{M}_{ij}$. We thus deduce an alternative series for C_{sub} built from A , A' and $i\mathcal{M}$ s, all connected by \mathcal{F} s [Fig. 1(d)].

We stress that the analysis just performed is a straightforward generalization of the single channel analysis of Ref. [16]. All that has changed is that \mathcal{F} and \mathcal{M} are now 2×2 matrices in channel space, and A and A' vectors.

To proceed, we decompose A , A' , \mathcal{M} and \mathcal{F} in spherical harmonics, defining coefficients via

$$A_j(\hat{k}^*) \equiv \sqrt{4\pi} A_{j;\ell,m} Y_{\ell,m}(\hat{k}^*) \quad (20)$$

$$A'_j(\hat{k}^*) \equiv \sqrt{4\pi} A'_{j;\ell,m} Y_{\ell,m}^*(\hat{k}^*) \quad (21)$$

$$\mathcal{M}_{ij}(\hat{k}^*, \hat{k}'^*) \equiv 4\pi \mathcal{M}_{ij;\ell_1,m_1;\ell_2,m_2} Y_{\ell_1,m_1}(\hat{k}^*) Y_{\ell_2,m_2}^*(\hat{k}'^*) \quad (22)$$

$$\begin{aligned} \mathcal{F}_{ij}(\hat{k}^*, \hat{k}'^*) \equiv \\ -\frac{1}{4\pi} F_{ij;\ell_1,m_1;\ell_2,m_2} Y_{\ell_1,m_1}(\hat{k}^*) Y_{\ell_2,m_2}^*(\hat{k}'^*), \end{aligned} \quad (23)$$

where a sum over all ℓ 's and m 's is implicit. The factors of 4π are present so that we match the conventions of Ref. [16]. They imply, for example, that for a purely s-wave amplitude, \mathcal{M} is the same in the two bases (for the 4π cancels with the two spherical harmonics). The kinematical factor F is given in Ref. [16] (aside from the above-noted factor of η_i) and takes the form³

$$\begin{aligned} F_{ij;\ell_1,m_1;\ell_2,m_2} &\equiv \delta_{ij} F_{i;\ell_1,m_1;\ell_2,m_2} \\ &= \delta_{ij} \eta_i \left[\frac{\text{Re } q_i^*}{8\pi E^*} \delta_{\ell_1 \ell_2} \delta_{m_1 m_2} \right. \\ &\quad \left. - \frac{i}{2E^*} \sum_{\ell,m} \frac{\sqrt{4\pi}}{q^{*\ell}} c_{\ell m}^P(q_i^{*2}) \int d\Omega Y_{\ell_1,m_1}^* Y_{\ell,m}^* Y_{\ell_2,m_2} \right]. \end{aligned} \quad (24)$$

² The result (14) is equivalent to Eqs. (41-42) of Ref. [16], although we have done some further manipulations to the last line of (14) to bring it into a matrix form. Also, we have included a factor of η_i in \mathcal{F} , rather than keeping it explicitly as in Ref. [16].

³ An additional difference from Ref. [16] is the appearance of $\text{Re } q_i^*$ rather than q^* . This is discussed in the next section.

Here the volume-dependence enters through the sums⁴

$$c_{\ell m}^P(q^{*2}) = \frac{1}{L^3} \sum_{\vec{k}} \frac{\omega_k^*}{\omega_k} \frac{e^{\alpha(q^{*2}-k^{*2})}}{q^{*2}-k^{*2}} k^{*\ell} \sqrt{4\pi} Y_{\ell,m}(\hat{k}^*) - \delta_{\ell 0} \mathcal{P} \int \frac{d^3 k^*}{(2\pi)^3} \frac{e^{\alpha(q^{*2}-k^{*2})}}{q^{*2}-k^{*2}}, \quad (25)$$

with $\omega_k = \sqrt{\vec{k}^2 + m_i^2}$ being the energy of a particle with momentum \vec{k} , and ω_k^* the energy after boosting to the CM frame. The properties of these sums are discussed in Ref. [16].

We are now in a position to write down the final result. The series indicated in Fig. 1(d) gives

$$C_{\text{sub}}(P) = - \sum_{n=0}^{\infty} A' F [-i\mathcal{M}F]^n A, \quad (26)$$

$$= -A' \frac{1}{F^{-1} + i\mathcal{M}} A. \quad (27)$$

Here all indices are left implicit and may be restored in the obvious way. For example,

$$A' F \mathcal{M} F A = A'_{ij;\ell_1,m_1} F_{ij;\ell_1,m_1;\ell_2,m_2} \mathcal{M}_{jk;\ell_2,m_2;\ell_3,m_3} F_{kl;\ell_3,m_3;\ell_4,m_4} A_{l,\ell_4,m_4}. \quad (28)$$

As C_{∞} is regular in the region of E^* that we consider (below $4M_{\pi}$), the poles in C_L must match the poles in C_{sub} . The desired quantization condition is then just that the matrix between A' and A have a divergent eigenvalue. This may be written as

$$\det(F^{-1} + i\mathcal{M}) = 0, \quad (29)$$

where we recall that the matrices now act in the product of the two-dimensional channel space and the infinite-dimensional angular-momentum space. More precisely, F is diagonal in channel space but has off-diagonal elements between different angular momentum sectors (as allowed by the symmetries of the cubic box and the momentum \vec{P}), while \mathcal{M} is diagonal in angular momentum but off-diagonal in channel space.

Equation (29) is the main result of this section. It has exactly the same form as that for the single channel given in Ref. [16] (aside from the change of notation in which symmetry factors are contained in F rather than kept explicit). The generalization to more than two two-particle channels is now immediate. As long as E^* is kept below the four particle threshold of the lightest particle the arguments above go through in the same manner.

One need only extend the values of the channel indices, taking care to include the appropriate symmetry factor η_j for each channel. The final result then has exactly the form of Eq. (29).

To make the formal expression (29) useful in practice one assumes that there is some ℓ_{max} , above which the partial wave amplitudes are negligible

$$\mathcal{M}_{ij}^{\ell > \ell_{\text{max}}} = 0. \quad (30)$$

One can then show that, although F couples $\ell \leq \ell_{\text{max}}$ to $\ell > \ell_{\text{max}}$, the projection contained in \mathcal{M} is sufficient to collapse the required determinant to that in the $\ell \leq \ell_{\text{max}}$ subspace. The argument for this result is given for one channel in Ref. [16] and generalizes trivially to the multiple channel case. Thus one finds that Eq. (29) still holds, but with \mathcal{M} and F now understood to be finite dimensional matrices both in channel space and in the partial wave basis, with ℓ running up to ℓ_{max} .

To conclude this section we comment briefly on two generalizations of the result. We first consider the case when not just a single σ but rather a set of operators $\{\sigma^a\}$ is of interest. This is likely to be the case in practice since multiple operators may be needed to find combinations with good overlaps with the finite-volume eigenstates. If there are n such operators, then C_L generalizes to an $n \times n$ matrix:

$$C_L^{ab}(P) = \int_{L;x} e^{i(-\vec{P} \cdot \vec{x} + Ex^0)} \langle 0 | \sigma^a(x) \sigma^{\dagger b}(0) | 0 \rangle. \quad (31)$$

The generalization of Eq. (27) is effected by replacing A' with an $n \times 2$ matrix

$$(A'_1 \ A'_2) \longrightarrow \begin{pmatrix} A'^{a=1}_1 & A'^{a=1}_2 \\ A'^{a=2}_1 & A'^{a=2}_2 \\ \vdots & \vdots \end{pmatrix} \quad (32)$$

and A with a $2 \times n$ matrix

$$\begin{pmatrix} A_1 \\ A_2 \end{pmatrix} \longrightarrow \begin{pmatrix} A^{b=1}_1 & A^{b=2}_1 & \dots \\ A^{b=1}_2 & A^{b=2}_2 & \dots \end{pmatrix}. \quad (33)$$

The key point, however, is that the matrix between A' and A is unchanged, so that the quantization condition (29) is unaffected. This is as expected, since the operators used to couple to states cannot affect the eigenstates themselves.

The second generalization is to the case of non-degenerate particles. The expressions given above remain valid as long as one makes three changes. First, the symmetry factors η_i become unity for all non-degenerate channels. Second, q_i^* in Eqs. (24) is replaced by the solution of

$$E^* = \sqrt{q_i^{*2} + M_{ia}^2} + \sqrt{q_i^{*2} + M_{ib}^2}, \quad (34)$$

which is the CM momentum when the channel contains particles of masses M_{ia} and M_{ib} . Third, when evaluating

⁴ We are slightly abusing the notation here for the sake of clarity. $c_{\ell m}^P$ depends not only on q^{*2} but also on m_i , but we keep the latter dependence implicit. The dependence is made explicit at the end of this section.

$c_{\ell m}^P$ using Eq. (25), one should use one of the masses M_{ia} or M_{ib} when determining ω_k , ω_k^* and \vec{k}^* . One can show that both choices lead to the same result.

The third change emphasizes that the kinematic functions $c_{\ell m}^P$ depend not only on q_i^* but also on the particle masses. This can be made explicit by rewriting them in terms of a generalization of the zeta-function introduced in Ref. [15]. The result is [26–29]

$$c_{\ell m}^P(q^{*2}) = -\frac{\sqrt{4\pi}}{\gamma L^3} \left(\frac{2\pi}{L}\right)^{\ell-2} \mathcal{Z}_{\ell m}^P[1; (q^* L/2\pi)^2], \quad (35)$$

$$\mathcal{Z}_{\ell m}^P[s; x^2] = \sum_{\vec{n}} \frac{r^\ell Y_{\ell m}(\hat{r})}{(r^2 - x^2)^s}, \quad (36)$$

where $\gamma = E/E^*$, \vec{n} runs over integer vectors, and \vec{r} is obtained from \vec{n} by $r_{\parallel} = \gamma^{-1}[n_{\parallel} - c\vec{n}_P]$ and $r_{\perp} = n_{\perp}$, where parallel and perpendicular are relative to \vec{P} , and $2c = (1 + (M_{1a}^2 - M_{1b}^2)/E^{*2})$. The sum in $\mathcal{Z}_{\ell m}$ can be regulated by taking $s > (3 + \ell)/2$ and then analytically continuing to $s = 1$. This shows that mass dependence enters through the difference⁵ $M_{ia}^2 - M_{ib}^2$. One can derive (35) by generalizing the method used for the degenerate case in Ref. [16].

III. MULTIPLE-CHANNEL QUANTIZATION CONDITION FOR S-WAVE SCATTERING

For the remainder of this article we focus on the simplest case, $\ell_{max} = 0$, in which only s-wave scattering is significant. In this section we determine the explicit form for the finite-volume quantization condition when there are two channels. We also present compact forms for the condition when an arbitrary number of two particle channels are open.

With only s-wave scattering, the two channel quantization condition takes the form

$$[(F_1^s)^{-1} + i\mathcal{M}_{11}^s][(F_2^s)^{-1} + i\mathcal{M}_{22}^s] - [i\mathcal{M}_{12}^s][i\mathcal{M}_{21}^s] = 0, \quad (37)$$

⁵ The apparent lack of symmetry under the interchange $M_{ia} \leftrightarrow M_{ib}$ can be understood as follows. One can show that $\mathcal{Z}_{\ell m}^P \rightarrow (-)^{\ell} \mathcal{Z}_{\ell m}^P$ under this interchange (so that for degenerate masses the zeta-functions for odd ℓ vanish [15]). This sign flip for odd ℓ must hold also for the $c_{\ell m}^P$, and it does because the interchange of masses leads to $\vec{k}^* \rightarrow -\vec{k}^*$ at the pole. The sign flip is canceled in the expression for \mathcal{F} , Eq. (23), since the product $Y_{\ell_1, m_1}(\vec{k}^*) Y_{\ell_2, m_2}^*(\vec{k}^{*'})$ also changes sign. This is because, when ℓ is odd, the integral over $d\Omega$ in the definition of F , Eq. (24), enforces that $\ell_1 + \ell_2$ is odd. The overall effect is that the quantization condition is symmetric under mass interchange, as it must be.

where

$$F_i^s = \eta_i \left[\frac{\text{Re } q_i^*}{8\pi E^*} - \frac{i}{2E^*} c_i^P \right] \quad (38)$$

$$c_i^P \equiv c^P(q_i^{*2}) \equiv c_{00}^P(q_i^{*2}), \quad (39)$$

and the superscript on F and \mathcal{M} is a reminder that only $\ell = 0$ contributes.

To simplify Eq. (37), and in particular to re-express it as an equation between real quantities, it is useful to recall first the single-channel analysis. This has the additional benefit of showing how the two-channel result collapses to the known single-channel result in the appropriate kinematic regime, namely

$$2M_{\pi} < E^* < 2M_K. \quad (40)$$

In this regime q_2^* becomes imaginary, and the second channel contributes negligibly because c^P [Eq. (25)] becomes exponentially volume-suppressed and $\text{Re } q^*$ in F_2 [Eq. (24)] vanishes.⁶ Sending $F_2 \rightarrow 0$ we find that the quantization condition becomes

$$[\mathcal{M}_{11}^s]^{-1} = \eta_1 \left[-\frac{iq_1^*}{8\pi E^*} - \frac{1}{2E^*} c^P(q_1^{*2}) \right]. \quad (41)$$

Note that the pion momentum q_1^* is real for the energy region considered.

Naively one might think that Eq. (41) gives two conditions, the separate vanishing of the real and imaginary parts. This is not the case, however, because the vanishing of the imaginary part is a volume-independent condition which is guaranteed to hold by the unitarity of the S -matrix. This can be seen by expressing \mathcal{M} in terms of the real phase shift $\delta(q^*)$,

$$\mathcal{M}_{11}^s = \frac{8\pi E^*}{\eta_1 q_1^*} \left[\frac{e^{2i\delta(q_1^*)} - 1}{2i} \right] = \left[\frac{\eta_1 q_1^*}{8\pi E^*} [\cot \delta(q_1^*) - i] \right]^{-1}. \quad (42)$$

Here $e^{2i\delta}$ is the one dimensional unitary S -matrix in the partial wave basis. Given Eq. (42), it is manifest that the imaginary part of Eq. (41) holds automatically. The real part of (41) then gives the moving frame generalization of the Lüscher result in the familiar partial wave form [13, 16, 17]

$$\tan \delta(q_1^*) = -\tan \phi^P(q_1^*), \quad (43)$$

where

$$\tan \phi^P(q^*) = \frac{q^*}{4\pi} [c^P(q^{*2})]^{-1}. \quad (44)$$

⁶ The appearance of $\text{Re } q^*$ rather than q^* in F_i can be understood by reviewing the derivation of F in Ref. [16]. The term enters as the difference between principal part and $i\epsilon$ prescriptions. When q^* is imaginary there is no pole and different ways of regulating give the same result.

We now return to the CM energies for which both channels are open, $2M_K < E^* < 4M_\pi$, and generalize Eq. (43). The first step is to recall the relationship between the scattering amplitude and the S -matrix. Unitarity implies that

$$\mathcal{M}^s - \mathcal{M}^{s\dagger} = i\mathcal{M}^{s\dagger} P^2 \mathcal{M}^s, \quad (45)$$

where P^2 is a diagonal matrix containing the phase-space factors, whose square root is

$$P = \frac{1}{\sqrt{4\pi E^*}} \begin{pmatrix} \sqrt{\eta_1 q_1^*} & 0 \\ 0 & \sqrt{\eta_2 q_2^*} \end{pmatrix}. \quad (46)$$

We note that, when expressed in terms of q^* , the form of P is still valid if the two particles in the channel are non-degenerate. We also note that the form (45) holds for an arbitrary number of two-particle, s-wave channels, with P generalized in the obvious way.

The solution to the unitarity relation is

$$i\mathcal{M}^s = P^{-1} (S^s - 1) P^{-1} \quad (47)$$

where S^s is a dimensionless, unitary 2×2 matrix. To proceed, we need to parametrize S^s . First we note that S^s can be taken to be symmetric. This is because of the T-invariance of the strong interactions, together with the fact that angular momentum eigenstates have definite T-parity (in our case, positive). Thus in the 2×2 case, S^s is determined by three real parameters. We use the ‘‘eigenphase convention’’ of Blatt and Biedenharn [30],

$$S^s = \begin{pmatrix} c_\epsilon & -s_\epsilon \\ s_\epsilon & c_\epsilon \end{pmatrix} \begin{pmatrix} e^{2i\delta_\alpha} & 0 \\ 0 & e^{2i\delta_\beta} \end{pmatrix} \begin{pmatrix} c_\epsilon & s_\epsilon \\ -s_\epsilon & c_\epsilon \end{pmatrix}, \quad (48)$$

where the notation $s_x = \sin x$ and $c_x = \cos x$ will be used throughout. The three real parameters δ_α , δ_β , and ϵ generalize the single δ which appears in the one channel case. The parameter ϵ quantifies the mixing between the mass eigenstates of channels one and two (the pions and kaons) and the S -matrix eigenstates. The phases δ_α and δ_β are, for arbitrary ϵ , associated with both channels. Of course, in the limit $\epsilon \rightarrow 0$ they reduce, respectively, to the phase shifts of pion and kaon elastic scattering.

Substituting the form of S^s into Eq. (47) and then placing this in Eq. (37) and simplifying, we deduce⁷

$$\begin{aligned} & [\tan \delta_\alpha + \tan \phi^P(q_1^*)] [\tan \delta_\beta + \tan \phi^P(q_2^*)] \\ & + \sin^2 \epsilon [\tan \delta_\alpha - \tan \delta_\beta] [\tan \phi^P(q_1^*) - \tan \phi^P(q_2^*)] \\ & = 0. \end{aligned} \quad (49)$$

⁷ We emphasize that the physical content of Eq. (49), namely that there is a relation between scattering amplitudes and energy levels, does not depend on the parametrization chosen for the matrix S^s . This is clear either from Eq. (37) or from Eq. (58) below. An advantage of our choice of parametrization is that it shows that Eq. (37) only implies one real condition (rather than two), an observation which must hold for any parameterization. We also note that the freedom to independently change the phases of $\pi\pi$ and $K\bar{K}$ states, which leads to $S^s \rightarrow U^\dagger S^s U$, with U a diagonal unitary matrix, does not change the quantization condition, as can be seen most easily from Eq. (58) below.

This is the main result of this section. One can use it in one of two ways: to predict the spectrum given knowledge of the scattering amplitude from experiment or a model, or to determine the S -matrix parameters from a lattice calculation of the spectrum. In the former case, we note that all quantities appearing in (49), i.e. δ_α , δ_β , ϵ , q_i^* and ϕ^P , are functions of E^* . One can thus search, at given spatial extent L and total momentum \vec{P} , for values of E^* which satisfy Eq. (49). If the condition holds for a particular E_k^* , then

$$E_k(L; \vec{n}_P) = \sqrt{E_k^{*2} + \vec{P}^2} \quad (50)$$

is in the spectrum of the finite-volume moving-frame Hamiltonian. Here we choose to write E_k as a function of \vec{n}_P rather than \vec{P} , since, in practice, it is the former quantity which is held fixed as one varies L .

The second use of (49) is the most relevant for the discussion in subsequent sections. For a given choice of E^* , one finds, through a lattice calculation, three pairs $\{L, \vec{n}_P\}$ for which there is a spectral line E_k such that E_k^* [defined in Eq. (50)] is equal to E^* . One could use a fixed \vec{n}_P and consider multiple spectral lines (the simplest choice conceptually), or use three different choices of \vec{n}_P (probably more practical since one would not need to determine so many excited levels). In either case, one ends up with three versions of Eq. (49), all containing the desired quantities $\delta_\alpha(E^*)$, $\delta_\beta(E^*)$ and $\epsilon(E^*)$, but having different values of the $\phi^P(q_j^*)$. Solving these equations one determines, rather than the angles themselves, the quantities $\tan \delta_\alpha$, $\tan \delta_\beta$, and $\sin^2 \epsilon$ at CM energy E^* . For our discussion we therefore restrict

$$\delta_{\alpha,\beta} \in [-\pi/2, \pi/2] \quad \text{and} \quad \epsilon \in [0, \pi/2]. \quad (51)$$

Having determined the restricted phases over a range of energies, one can afterward relax the constraints in order to build continuous curves as a function of energy. We direct the reader to Refs. [22, 23] for discussion of other methods for extracting the three scattering parameters.

We emphasize that Eq. (49) has a very intuitive form. If $\delta_\alpha = \delta_\beta$ or $m_1 = m_2$ or $\epsilon = 0$ then the second line vanishes and the result reduces to two copies of the one channel quantization condition [Eq. (43)]. To see that this makes sense, note that for identical phase shifts, the ϵ matrix commutes through the phase matrix and we recover two uncoupled channels. Similarly if the masses are degenerate then the eigenstates of the S -matrix will also be mass eigenstates leading to the decoupled form. Finally, the decoupling for $\epsilon = 0$ is an obvious property of the parametrization [Eq. (48)].

An alternative solution to the unitarity relation (45) can be given in terms of the K -matrix used in Ref. [22]. Specifically, (45) is satisfied if

$$(\mathcal{M}^s)^{-1} = M - iP^2/2, \quad (52)$$

with M any real symmetric 2×2 matrix. If we set

$$M = \frac{1}{8\pi E^*} \|\sqrt{\eta}\| K^{-1} \|\sqrt{\eta}\|, \quad (53)$$

[where double bars denote a diagonal matrix, so that $\|\eta\| = \text{diag}(\sqrt{\eta_1}, \sqrt{\eta_2})$, and further set $\vec{P} = 0$, then one can show that the two-channel quantization condition given above can be manipulated into the form given in Eq. (3.5) of Ref. [22] in terms of the real, symmetric matrix K .

We now generalize Eq. (49) to N s-wave channels. As noted above, the form of the unitarity relation (45) holds for any N , and the same is true for its solution (47). In the latter, the N channel S -matrix can be parametrized as⁸

$$S = R^{-1} \|e^{2i\delta}\| R, \quad (54)$$

with R an $SO(N)$ matrix, and

$$\|e^{2i\delta}\| = \text{diag}[e^{2i\delta_\alpha}, e^{2i\delta_\beta}, \dots]. \quad (55)$$

Together with Eqs. (54) and (55) one needs the $N \times N$ generalization of F , which has been discussed in the previous section. From these definitions one can straightforwardly work out the quantization condition for N coupled channels.

We conclude this section by describing two additional ways of writing the quantization condition, both of which make the higher channel generalization especially clear. Observe first that, for any number of open channels,

$$F^{-1} = P^{-1} \|1 - e^{-2i\phi}\| P^{-1}. \quad (56)$$

Combining this with (47), it follows that

$$F^{-1} + i\mathcal{M} = P^{-1} [S - \|e^{-2i\phi}\|] P^{-1}. \quad (57)$$

Since P^{-1} has no singularities in the kinematic regime we consider, the quantization condition can be rewritten as

$$\det [S - \|e^{-2i\phi}\|] = 0. \quad (58)$$

This form shows that the symmetry factors cancel from the quantization condition in general. Although Eq. (58) looks like it will lead to one complex and thus two real conditions, it turns out that it leads only to a single real condition. This follows from the identity

$$\begin{aligned} \|1 + it_\phi\| \times [S - \|e^{-2i\phi}\|] \times [R^{-1} \|1 - it_\delta\| R] \\ = 2i [R^{-1} \|t_\delta\| R + \|t_\phi\|], \end{aligned} \quad (59)$$

where $t_x = \tan x$. It gives a manifestly real rewriting of the quantization condition,

$$\det [R^{-1} \|t_\delta\| R + \|t_\phi\|] = 0. \quad (60)$$

This form leads directly to the result (49) in the two channel case, and collapses to the single-channel result (43) for any channel that decouples from the rest. If any of the channels contain non-degenerate particles, this enters only through the values of the kinematic functions t_ϕ , as discussed in the previous section.

IV. MULTIPLE CHANNEL EXTENSION OF THE LELLOUCH-LÜSCHER FORMULA

Having found the two channel quantization condition, we are now in a position to work out the two channel generalization of the LL formula which relates weak matrix elements in finite and infinite volume. The derivation follows the original work by Lellouch and Lüscher, Ref. [18], which was extended to a moving frame by Refs. [16, 17].

We begin by introducing a third channel which is decoupled from the original two. This contains a single particle, which we call a D -meson, whose mass satisfies

$$M_D > 2M_\pi, 2M_K. \quad (61)$$

We next introduce a weak perturbation to the Hamiltonian density

$$\mathcal{H}(x) \rightarrow \mathcal{H}(x) + \lambda \mathcal{H}_W(x), \quad (62)$$

where λ is a parameter which can be varied freely and can, in particular, be taken arbitrarily small. The perturbation \mathcal{H}_W is defined to couple channels one and two (pions and kaons) to the third (D -meson) and nothing more. It is convenient to choose it to be invariant under time reversal (T) symmetry. The generalization to perturbations which are not T invariant is described at the end of the section.

Consider now the finite volume spectrum, first in the absence of the perturbation. The spectrum of two-particle states with $\vec{P} = 2\pi\vec{n}_P/L$ is determined by Eq. (49). It is L -dependent and L can therefore be tuned to make one of the levels, call it k_D , degenerate with the energy of a single (moving) D meson

$$E_{k_D} = \sqrt{M_D^2 + \vec{P}^2} \quad (63)$$

With L fixed in this way, we now turn on the weak interaction. At leading order in degenerate perturbation theory this changes the energies to

$$E^{(1)} = E^{(0)} \pm \lambda V |M_W| \quad (64)$$

where $V = L^3$, $E^{(0)} = E_{k_D}$, and the finite-volume matrix element is

$$M_W = {}_L\langle k_D | \mathcal{H}_W(0) | D \rangle_L. \quad (65)$$

The subscripts L on the states indicate that they are normalized to unity, unlike the relativistically normalized infinite volume states. Superscripts ⁽¹⁾ are used throughout

⁸ The remainder of this paper is limited to the s -wave, so we drop the superscript ^s hereafter.

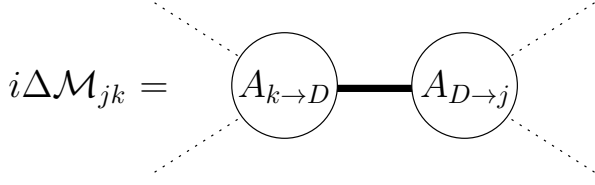


FIG. 2. The diagram giving rise to the amplitude perturbation $\Delta\mathcal{M}$ [See Eq. (69)].

this section to indicate that the quantity includes both the leading order and the $\mathcal{O}(\lambda)$ correction, while superscripts (0) indicate the unperturbed quantity. The effect of the perturbation may also be written in terms of the CM energy as

$$E^{*(1)} = M_D \pm \lambda \Delta E^* \quad (66)$$

$$\Delta E^* = \frac{E^{(0)} V |M_W|}{M_D}. \quad (67)$$

Of course, in addition to affecting the finite volume energy spectrum, the weak perturbation also changes the infinite volume scattering amplitudes. The leading order effect is generated by the diagram of Fig. 2, which gives

$$\mathcal{M}^{(1)} = \mathcal{M}^{(0)} \mp \lambda \Delta\mathcal{M} \quad (68)$$

with

$$\Delta\mathcal{M}_{j,k} = \frac{\langle j | \mathcal{H}_W(0) | D \rangle \langle D | \mathcal{H}_W(0) | k \rangle}{2E^{(0)} V |M_W|}. \quad (69)$$

The indices j and k run over the two two-particle channels. This perturbation may equivalently be represented through shifts in δ_α , δ_β and ϵ

$$\delta_\alpha^{(1)}(E^*) = \delta_\alpha^{(0)}(E^*) \pm \lambda \Delta\delta_\alpha(E^*) \quad (70)$$

$$\delta_\beta^{(1)}(E^*) = \delta_\beta^{(0)}(E^*) \pm \lambda \Delta\delta_\beta(E^*) \quad (71)$$

$$\epsilon^{(1)}(E^*) = \epsilon^{(0)}(E^*) \pm \lambda \Delta\epsilon(E^*), \quad (72)$$

The explicit forms of the perturbed phases are given in Eqs. (81)-(83) below.

The calculation now proceeds as follows. When the quantities

$$\delta_\alpha^{(0)}(E^*), \delta_\beta^{(0)}(E^*), \text{ and } \epsilon^{(0)}(E^*) \quad (73)$$

are placed in the quantization condition [Eq. (49)], the condition is satisfied by construction at $E^{*(0)} = M_D$. Alternatively if one places

$$\delta_\alpha^{(1)}(E^*), \delta_\beta^{(1)}(E^*), \text{ and } \epsilon^{(1)}(E^*) \quad (74)$$

into the same condition then it must be satisfied when evaluated at the perturbed CM energy $E^{*(1)}$, but only to linear order in λ . The constant order term in the λ expansion is just the unperturbed condition, and so it is

the vanishing of the $\mathcal{O}(\lambda)$ term that is of interest. The condition that this term vanish gives the relation between finite and infinite volume weak matrix elements that we are after.

The only detail left to discuss, before substituting into the quantization condition and expanding in λ , is the explicit forms of the amplitude corrections to δ_α , δ_β and ϵ . Before these are found it is useful to determine the constraints on the infinite volume matrix elements which arise from Watson's theorem. As shown in App. A, time reversal invariance and unitarity constrain the matrix elements to be such that the following two quantities are real:

$$v_1 = e^{-i\delta_\alpha} \left[\sqrt{q_1^* \eta_1} A_{D \rightarrow \pi\pi} c_\epsilon + \sqrt{q_2^* \eta_2} A_{D \rightarrow KK} s_\epsilon \right], \quad (75)$$

$$v_2 = e^{-i\delta_\beta} \left[-\sqrt{q_1^* \eta_1} A_{D \rightarrow \pi\pi} s_\epsilon + \sqrt{q_2^* \eta_2} A_{D \rightarrow KK} c_\epsilon \right]. \quad (76)$$

Here

$$A_{D \rightarrow \pi\pi} \equiv \langle \pi\pi | \mathcal{H}_W(0) | D \rangle, \quad (77)$$

and similarly for the $K\bar{K}$ case, normalized so that the decay rates to each channel are

$$\Gamma_{D \rightarrow j} = \frac{q_j^* \eta_j}{8\pi M_D^2} |A_{D \rightarrow j}|^2 = \frac{1}{2M_D} P_{jj}^2 |A_{D \rightarrow j}|^2. \quad (78)$$

This relation holds also if the particles in a channel are non-degenerate (requiring $\eta = 1$). All energy-dependent parameters in (75) and (76), i.e. δ_α , δ_β , ϵ and q_j^* , are to be evaluated at $E^* = M_D$.

The results (75) and (76) hold when the phases of the states are chosen so that the S -matrix is symmetric (as is possible given T invariance). This does not determine the signs of the two matrix elements, and these signs are unphysical. More precisely, the relative sign ambiguity is the same as the ambiguity in the sign of ϵ , so once we have fixed the latter to be positive, the relative sign is physical. The overall sign remains unphysical, and can be chosen, for example to set $v_1 \geq 0$,

Inverting the relations (75) and (76) yields

$$A_{D \rightarrow \pi\pi} = \frac{1}{\sqrt{q_1^* \eta_1}} [v_1 e^{i\delta_\alpha} c_\epsilon - v_2 e^{i\delta_\beta} s_\epsilon] \quad (79)$$

$$A_{D \rightarrow KK} = \frac{1}{\sqrt{q_2^* \eta_2}} [v_1 e^{i\delta_\alpha} s_\epsilon + v_2 e^{i\delta_\beta} c_\epsilon]. \quad (80)$$

Inserting these in $\Delta\mathcal{M}$, Eq. (69), and using the relation between \mathcal{M} and S , Eq. (47), and the parametrization of S , Eq. (48), we find that perturbations to δ_α , δ_β and ϵ are real. This is a consistency check on the calculation (or an alternative derivation of the Watson's theorem constraint). Specifically, we find

$$\Delta\delta_\alpha = -\mathcal{N} v_1^2 \quad (81)$$

$$\Delta\delta_\beta = -\mathcal{N} v_2^2 \quad (82)$$

$$\Delta\epsilon = -\mathcal{N} \frac{v_1 v_2}{c_\alpha c_\beta (t_\alpha - t_\beta)} \quad (83)$$

where $t_\alpha = \tan \delta_\alpha$, etc., and

$$\mathcal{N} = \frac{1}{16\pi E^{(0)} M_D V |M_W|}. \quad (84)$$

We now have all the ingredients to substitute into the quantization condition and determine the LL generalization. We emphasize that, when the expansion in λ is performed, δ_α , δ_β and ϵ each contribute both from the amplitude corrections of Eqs. (81)-(83) and from the shift in the energy, (66). The other contributions arise from the energy dependence of $\phi_i = \phi^P(q_i^*)$. Substituting and simplifying, we find the main result of this section

$$\mathcal{C}_1 v_1^2 + \mathcal{C}_2 v_2^2 + \mathcal{C}_{12} v_1 v_2 = \mathcal{C}_{M^2} |M_W|^2 \quad (85)$$

where

$$\mathcal{C}_1 = \frac{\pi}{16} \frac{t_1 + t_2 + 2t_\beta + (t_2 - t_1)(1 - 2s_\epsilon^2)}{c_\alpha^2} \quad (86)$$

$$\mathcal{C}_2 = \frac{\pi}{16} \frac{t_1 + t_2 + 2t_\alpha + (t_1 - t_2)(1 - 2s_\epsilon^2)}{c_\beta^2} \quad (87)$$

$$\mathcal{C}_{12} = \frac{\pi}{4} (t_1 - t_2) \frac{s_\epsilon c_\epsilon}{c_\alpha c_\beta} \quad (88)$$

$$\begin{aligned} \mathcal{C}_{M^2} = & \frac{\pi^2 M_D V^2 (E^{(0)})^2}{2} \left[\frac{t'_1}{q_1^*} (t_2 + t_\beta + (t_\alpha - t_\beta) s_\epsilon^2) \right. \\ & + \frac{t'_2}{q_2^*} (t_1 + t_\alpha + (t_\beta - t_\alpha) s_\epsilon^2) \\ & + \frac{4t'_\alpha}{M_D} (t_2 + t_\beta + (t_1 - t_2) s_\epsilon^2) \\ & + \frac{4t'_\beta}{M_D} (t_1 + t_\alpha + (t_2 - t_1) s_\epsilon^2) \\ & \left. + \frac{4s_\epsilon'^2}{M_D} (t_1 - t_2)(t_\alpha - t_\beta) \right], \end{aligned} \quad (89)$$

and where we use the additional notation

$$t_i = \tan \phi^P[q_i^*]. \quad (90)$$

All quantities are evaluated at the D mass, and we have dropped the superscript (0) . The primes on ϕ_i indicate derivatives with respect to q_i^* while those on δ_α , δ_β and ϵ indicate derivatives with respect to E^* . In each case, these are the natural variables on which the quantities depend. We have checked that this formula reduces to (two copies of) the single-channel LL result if $\epsilon \rightarrow 0$.

We now describe how the result (85) can be used in practice. A lattice calculation yields the finite-volume matrix element $|M_W|$, and the aim is to determine the infinite-volume matrix elements $A_{D \rightarrow \pi\pi}$ and $A_{D \rightarrow KK}$. Using the generalized quantization condition (49) for three different spectral lines (all chosen to have $E^* = M_D$) one can determine δ_α , δ_β and ϵ as described in the previous section. Repeating the procedure at a slightly different energy allows a numerical determination of the

required derivatives. One now evaluates $|M_W|$ at the degenerate point on one of the spectral lines. The knowledge of the S -matrix parameters and their derivatives, together with the value of L , allows one to calculate the values of the four \mathcal{C} 's [Eqs. (86)-(89)]. Combined with the value of $|M_W|$, one then finds from Eq. (85) a quadratic constraint on v_1 and v_2 . Repeating the procedure for a second spectral line gives an independent constraint, which allows for the determination of v_1 and v_2 up to a two-fold ambiguity corresponding to the unknown relative sign. Finally, repeating for a third spectral line resolves the sign ambiguity. With v_1 and v_2 determined in this way, one can obtain the infinite-volume matrix elements using Eqs. (79) and (80). Although this procedure is rather elaborate, we note that (for the case of two channels) three spectral lines are needed both for the determination of the parameters of the S -matrix and of the LL factors.

We conclude this section by commenting that Eq. (85) factors as

$$\text{sgn}(\mathcal{C}_1)(c_1 v_1 + c_2 v_2)^2 = \mathcal{C}_{M^2} |M_W|^2 \quad (91)$$

where

$$c_1 = \sqrt{|\mathcal{C}_1|} \quad c_2 = \text{sgn}[\mathcal{C}_1 \mathcal{C}_{12}] \sqrt{|\mathcal{C}_2|}. \quad (92)$$

The only new information encoded in Eqs. (91) and (92) relative to Eq. (85) is that

$$4\mathcal{C}_1 \mathcal{C}_2 = \mathcal{C}_{12}^2, \quad (93)$$

which can be shown to hold by applying Eq. (49) to Eqs. (86)-(88). Although the factorized form (91) is simpler, it does not reduce the number of values of L that are needed because there remains a sign ambiguity (from the square root) at each L . What it does make clear, however, is that the generalized LL condition will fail when the signs of \mathcal{C}_1 and \mathcal{C}_{M^2} are opposite. Presumably this cannot happen for physical values of the phase shifts. We stress that this issue also arises in the original one-channel set-up, where the LL formula only makes sense if

$$\frac{d(\delta + \phi^P)}{dq^*} > 0. \quad (94)$$

We return to these sign constraints in the next section.

The form (91) also allows one to write the LL condition as a factored form in terms of the desired matrix elements,

$$|c_\pi A_{D \rightarrow \pi\pi} + c_K A_{D \rightarrow KK}|^2 = |\mathcal{C}_{M^2}| |M_W|^2, \quad (95)$$

where c_π and c_K are complex, and can be determined from the above results. As this equality holds for any T-invariant form of weak perturbation and for any decay particle, it must imply a relation between finite and infinite volume states

$$L \langle k_D | \propto c_\pi \langle \pi\pi, \text{out} | + c_K \langle K\bar{K}, \text{out} | + \dots \quad (96)$$

Here the ellipsis indicates the $\pi\pi$ and $K\bar{K}$ states of higher angular momentum which are needed to satisfy the periodic boundary conditions. Indeed, as noted in the original derivation of Ref. [18], the use of the D -meson is simply a trick to obtain the normalization factors.⁹ It follows that Eq. (95) must also hold for perturbations which are not T-invariant.

The appearance of the linear combination in Eq. (96) can be better understood from an alternative derivation of the LL formula, to which we now turn.

V. ALTERNATIVE DERIVATION OF LELLOUCH-LÜSCHER FORMULA

In this section we present a different derivation of the two channel LL relation which has the following advantages: (a) it does not require determining the shifts $\Delta\delta_\alpha$, $\Delta\delta_\beta$ and $\Delta\epsilon$, but rather works directly with the change in \mathcal{M} ; (b) it gives one directly a condition with the factored form, proportional to the left hand side of Eq. (95); (c) it allows one to rewrite the LL condition in a simpler form in which the only inputs required are the derivatives of the energies with respect to L along the three spectral lines. This form is likely to be more practical.

We work directly with the condition $\det(F^{-1} + i\mathcal{M}) = 0$, and keep results for general number of channels, N , as far as possible. We begin by defining

$$\mathcal{X} = F^{-1} + i\mathcal{M} \quad (97)$$

$$\mathcal{Y} = S - \|e^{-2i\phi}\|. \quad (98)$$

and recall from Eq. (57) that

$$\mathcal{X} = P^{-1}\mathcal{Y}P^{-1}. \quad (99)$$

The quantization condition $\det \mathcal{X} = 0$ is equivalent to \mathcal{X} having an eigenvector with vanishing eigenvalue. We label this eigenvector \vec{e}^X . Note also that the symmetry of \mathcal{X} implies $(\vec{e}^X)^{Tr} = \overleftarrow{e}^X$ is a left eigenvector, also with zero eigenvalue.

Now we can formulate the LL condition in a relatively compact form. As above, let $\mathcal{M}^{(0)}$ be the scattering amplitude at CM energy $E^* = M_D$. Similarly, let $F^{(0)}$ be the finite-volume factor at this CM energy and for one of the values of box size L for which the quantization condition holds. Then for

$$\mathcal{X}^{(0)} \equiv (F^{(0)})^{-1} + i\mathcal{M}^{(0)}, \quad (100)$$

we have

$$\overleftarrow{e}^X \mathcal{X}^{(0)} \vec{e}^X = 0. \quad (101)$$

Now, while holding L fixed, we change the energy by $\pm\lambda\Delta E = \pm\lambda V|M_W|$ and change \mathcal{M} to $\mathcal{M}^{(0)} \mp \lambda\Delta\mathcal{M}$, and require that the quantization condition still hold. Thus we have, to linear order in λ ,

$$\det(\mathcal{X}^{(0)} + \lambda\Delta\mathcal{X}) = 0, \quad (102)$$

where

$$\Delta\mathcal{X} = \pm\Delta E \frac{\partial\mathcal{X}}{\partial E} \Big|_L \mp i\Delta\mathcal{M}. \quad (103)$$

It follows that there must be a new eigenvector of the form

$$\vec{e}^X + \lambda\Delta\vec{e}^X \quad (104)$$

which is annihilated by the perturbed matrix. From the $\mathcal{O}(\lambda)$ term in

$$[\overleftarrow{e}^X + \lambda\Delta\overleftarrow{e}^X] [\mathcal{X}^{(0)} + \lambda\Delta\mathcal{X}] [\vec{e}^X + \lambda\Delta\vec{e}^X] = 0, \quad (105)$$

we deduce

$$\overleftarrow{e}^X \Delta\mathcal{X} \vec{e}^X = 0. \quad (106)$$

Using the explicit form of $\Delta\mathcal{X}$ this becomes

$$\Delta E \overleftarrow{e}^X \frac{\partial\mathcal{X}}{\partial E} \Big|_L \vec{e}^X = \overleftarrow{e}^X i\Delta\mathcal{M} \vec{e}^X, \quad (107)$$

where the derivative is evaluated at $E^* = M_D$.

We can slightly simplify this result by expressing the left hand side in terms of \mathcal{Y} rather than \mathcal{X} , and thus removing factors of P^{-1} . The point is that, when the derivative acts on the P^{-1} factors in \mathcal{X} , the contribution to the left hand side vanishes, since one can still act (either to the left or the right) on the zero-eigenvector. Thus we can rewrite the condition in terms of the zero eigenvector of \mathcal{Y} , which is

$$\vec{e}^Y = P^{-1}\vec{e}^X. \quad (108)$$

The new form is

$$\Delta E \overleftarrow{e}^Y \frac{\partial\mathcal{Y}}{\partial E} \Big|_L \vec{e}^Y = \overleftarrow{e}^X [i\Delta\mathcal{M}] \vec{e}^X. \quad (109)$$

We now focus on the 2×2 case. To proceed, we need the explicit form for \vec{e}^Y , which is given, up to an overall normalization factor, by

$$\vec{e}^Y = \begin{bmatrix} 1 \\ ze^{i(\phi_2 - \phi_1)} \end{bmatrix} \quad (110)$$

⁹ In the one-channel case, an alternative line of argument has been developed for obtaining the LL relation, based on matching the density of two-particle states in finite and infinite volumes [31]. In the present case, we do not see how to use this approach to determine the relative normalization, c_K/c_π , of the two components in the finite volume state. Thus we think that this approach could provide only a consistency check.

where z is the real quantity

$$z = t_\epsilon \frac{\sin(\delta_\beta + \phi_1)}{\sin(\delta_\beta + \phi_2)}. \quad (111)$$

It is clear from the form of Eq. (109) and the relation (108) that the normalization of \vec{e}^Y is irrelevant and so we have chosen a relatively simple unnormalized form.

We evaluate the right hand side of Eq. (109) using the form of $\Delta\mathcal{M}$, Eq. (69). It is immediately apparent that the result factorizes, given that $\Delta\mathcal{M}$ is an outer product. This will hold for all N . In the $N = 2$ case we have

$$\overleftarrow{e}^X [i\Delta\mathcal{M}] \vec{e}^X = ie^{-2i\phi_1} \frac{M_\infty^2}{8\pi M_D E^{(0)} V |M_W|}, \quad (112)$$

where

$$M_\infty = e^{i\phi_1} \sqrt{q_1^* \eta_1} A_{D \rightarrow \pi\pi} + z e^{i\phi_2} \sqrt{q_2^* \eta_2} A_{D \rightarrow KK}. \quad (113)$$

Here we have used the assumed T-invariance of \mathcal{H}_W . We have pulled out the phase $e^{-2i\phi_1}$ so that M_∞ is real. Its reality is not obvious, but can be established using the results derived from Watson's theorem and given in App. A. In particular, an algebraic exercise shows that

$$M_\infty = \sin(\phi_1 - \phi_2) \left[-v_1 \frac{c_\epsilon}{\sin(\delta_\alpha + \phi_2)} + v_2 \frac{s_\epsilon}{\sin(\delta_\beta + \phi_2)} \right], \quad (114)$$

and we recall that the quantities v_1 and v_2 [defined above in Eqs. (75)-(76)] are real.

The result (113) makes clear that, for any choice of \mathcal{H}_W , one ends up with the matrix element to a given (complex) linear combination of $\langle \pi\pi |$ and $\langle K\bar{K} |$ states, since all the factors (ϕ_1 , ϕ_2 and z) are determined by $E^{(0)}$ and L . Indeed, what the LL method has allowed us to do is determine the coefficients of the s-wave $\langle \pi\pi |$ and $\langle K\bar{K} |$ components within the finite-volume state. As mentioned above, this decomposition has nothing to do with \mathcal{H}_W , and thus we can use the result for any \mathcal{H}_W , including one involving T-violation. By comparing the result (113) to the general decomposition of the finite-volume state, Eq. (96), we can read off the ratio of the coefficients,

$$\frac{c_K}{c_\pi} = e^{i(\phi_2 - \phi_1)} z \sqrt{\frac{q_2^* \eta_2}{q_1^* \eta_1}}. \quad (115)$$

It is interesting that the relative phase between c_K and c_π is determined by the kinematic phases ϕ_j . Given the form of $\Delta\mathcal{M}$, and the fact that, in Eq. (112), it is sandwiched between \overleftarrow{e}^X and \vec{e}^X , it follows that the zero eigenvector itself gives the relative size of the $\pi\pi$ and $K\bar{K}$ contributions:

$$\vec{e}^X \propto \begin{pmatrix} c_\pi \\ c_K \end{pmatrix}. \quad (116)$$

This illustrates in a direct way that the linear combination which appears is completely independent of the form of \mathcal{H}_W , since the eigenvector of \mathcal{X} knows nothing about this perturbation.

Having discussed the right hand side of Eq. (109) in some detail we now turn to the left. Specifically, we show that it is possible to write the left-hand side in terms of the derivative of the spectral energy with respect to L . To motivate this form, we first recall that the LL result of the previous section depends on δ_α , δ_β and ϵ and their derivatives, evaluated at $E^* = M_D$. As described in Sec. IV, the three S -matrix parameters may be determined, using Eq. (49), by finding three different pairs $\{L, \vec{n}_P\}$ for which there is a spectral line $E_k(L; \vec{n}_P)$ satisfying $E_k^*(L; \vec{n}_P) = M_D$ [see Eq. (50)]. Furthermore, by slightly changing the three L values, one can determine δ_α , δ_β and ϵ at slightly different energies and thus deduce the derivatives at M_D .

The point of reiterating these steps is to note that, since the lattice simulation actually gives the energy spectrum as a function of L , it would be preferable if the LL result could be rewritten directly in terms of the properties of the spectrum. In this way the extra step of separately working out the phase shifts and their derivatives would be avoided. This turns out to be possible, as we now show.

We use the quantization condition in the form $\det \mathcal{Y} = 0$. To stay on a spectral line $E_k(L; \vec{n}_P)$ as we vary E away from the moving frame D -meson energy $E^{(0)}$, we need to vary L in such a way that this condition remains fulfilled. We note that, while F depends on both E^* and L , S depends only on E^* . Thus we use E^* and L as independent variables. Then the condition to stay on a spectral line becomes

$$0 = \overleftarrow{e}^Y \left[\Delta E^* \frac{\partial \mathcal{Y}}{\partial E^*} \Big|_L + \Delta L \frac{\partial \mathcal{Y}}{\partial L} \Big|_{E^*} \right] \vec{e}^Y, \quad (117)$$

which leads to

$$\frac{dE_k^*}{dL} \Big|_{\text{line}} = - \frac{\overleftarrow{e}^Y \frac{\partial \mathcal{Y}}{\partial L} \vec{e}^Y}{\overleftarrow{e}^Y \frac{\partial \mathcal{Y}}{\partial E^*} \vec{e}^Y}. \quad (118)$$

Here, in the left-hand side, the subscript “line” indicates that the derivative is along a spectral line with fixed \vec{n}_P .

The key features of Eq. (118) are that the denominator on the right-hand side is, up to a simple overall factor, equal to the quantity appearing on the left hand side of the Eq. (109), while the numerator is a kinematic factor. Specifically, using

$$\overleftarrow{e}^Y \frac{\partial \mathcal{Y}}{\partial E^*} \vec{e}^Y = \frac{E^*}{E} \overleftarrow{e}^Y \frac{\partial \mathcal{Y}}{\partial E} \vec{e}^Y, \quad (119)$$

and

$$\frac{dE_k}{dL} \Big|_{\text{line}} = \frac{E_k^*}{E_k} \frac{dE_k^*}{dL} \Big|_{\text{line}} - \frac{\vec{P}^2}{EL} \quad (120)$$

(which follows since $E^2 = (E^*)^2 + (\vec{P}L)^2/L^2$ and because $\vec{P}L$ is fixed along the spectral line), we find

$$\overleftarrow{e}^Y \frac{\partial \mathcal{Y}}{\partial E} \overrightarrow{e}^Y = -2ie^{-2i\phi_1} \frac{\frac{\partial \phi_1}{\partial L} + z^2 \frac{\partial \phi_2}{\partial L}}{\frac{dE_k}{dL}|_{\text{line}} + \frac{\vec{P}^2}{E L}}. \quad (121)$$

Combining this with (109) and (112) we conclude

$$\frac{M_\infty^2}{16\pi M_D E^{(0)} V^2 |M_W|^2} = -\frac{\frac{\partial \phi_1}{\partial L} + z^2 \frac{\partial \phi_2}{\partial L}}{\frac{dE_k}{dL}|_{\text{line}} + \frac{\vec{P}^2}{E^{(0)} L}}. \quad (122)$$

We thus have found an alternative form of the LL relation which is simpler than Eq. (85), and also likely to be more practical.

The single channel version of (85) is instructive. It can be written, using Eq. (78), in terms of the decay rate:

$$\Gamma_{D \rightarrow \pi\pi} = \frac{2E^{(0)} V^2 |M_W|^2}{M_D} \left[\frac{-\frac{\partial \phi}{\partial L}}{\frac{dE_k}{dL}|_{\text{line}} + \frac{\vec{P}^2}{E^{(0)} L}} \right]. \quad (123)$$

This form holds both for identical and non-identical particles, with the symmetry factor being contained in Γ . It also sheds light on the sign constraints discussed in the previous section. The right-hand side must be positive. Based on numerical studies, we find that $\partial \phi / \partial L$ is always positive, implying that the denominator, which is proportional to dE_k^*/dL , must be negative.

The same holds for the two-channel result, Eq. (122). In order for the right-hand side to be positive, the denominator must be negative. Since we could do the LL analysis on almost any spectral line, this appears to imply that $dE_k^*/dL < 0$ in general. The only exception is for a state with E_k^* below the two particle threshold. Such a state occurs, for example, as the lowest energy state for $\vec{P} = 0$ if there is an attractive interaction. For such a state one has $dE_k^*/dL = dE_k/dL > 0$, i.e. of the “wrong” sign. But in this case the LL analysis does not apply, because the particle lies below threshold in infinite volume.

VI. CONCLUSIONS

We have presented two new results in this article. First, a field-theoretic derivation of the generalization of Lüscher’s quantization formula to the case of multiple strongly coupled two-particle channels (where the particles are spinless). Second, the generalization to multiple channels of the Lellouch-Lüscher formula relating finite-volume and infinite-volume matrix elements. We also have explained in some detail how, in the case of two channels, one can use these results to determine the infinite-volume decay amplitudes of a particle which is coupled by a weak interaction to the two-body channels.

As already noted in the introduction, this is but a step on the way toward our “dream” application, namely the calculation of $D^0 \rightarrow \pi\pi$ and $D^0 \rightarrow K\bar{K}$ amplitudes. To

achieve that goal, one will also need to include the channels with four or more pions. These are significant once one approaches the energy M_D . Work in this direction is underway.

An example where our formalism should be useful with minimal approximation is the determination of the isospin breaking in $K \rightarrow \pi\pi$ decays. Given the mass splitting between charged and neutral kaons, there are really two two-body channels to consider, and in this case the coupling to the four pion channel is very small and can reasonably be neglected.

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Appendix A: Two-channel Watson’s theorem

In this appendix we work out the consequences of Watson’s theorem for the phases of the matrix elements of interest, $\langle \pi\pi | \mathcal{H}_W(0) | D \rangle$ and $\langle K\bar{K} | \mathcal{H}_W(0) | D \rangle$. We assume at first that \mathcal{H}_W is T invariant, and describe the generalization to non-invariant Hamiltonians at the end. We closely follow the textbook presentation given in Ref. [32].

We consider the 3×3 S -matrix with the three states being the hypothetical D meson (at rest) and the s-wave $\pi\pi$ and $K\bar{K}$ states. We assume that we are in the kinematic regime described in the main text, so that the 3×3 S -matrix is unitary. Although we introduce a weak coupling between the D and the two particle states, so that the D is a resonance, its width is of second-order in the weak interaction and thus can be ignored at the linear order to which we work. Thus it is valid to treat it as an asymptotic state.

Watson’s theorem follows by breaking the S -matrix into a strong part $S^{(0)}$ and a weak part S^W . The strong part is T invariant, and, since we use states which have definite (positive) T-parity, can be taken to be symmetric. This fixes the phases of the $\pi\pi$ and $K\bar{K}$ states, though not their overall signs. Extending the dimensionless, strong-coupling S -matrix of Eq. (47) to include the D gives

$$S^{(0)} = \begin{pmatrix} 1 & 0 \\ 0 & S^s \end{pmatrix}, \quad (A1)$$

where 1 is the 1×1 identity and S^s is the 2×2 s-wave S -matrix given in (47). The weak part only contains couplings between the D and the two-particle states, and

in 3×3 notation is

$$S^W = \begin{pmatrix} 0 & S_{D,\pi\pi}^W & S_{D,KK}^W \\ S_{\pi\pi,D}^W & 0 & 0 \\ S_{KK,D}^W & 0 & 0 \end{pmatrix}. \quad (\text{A2})$$

The assumed T invariance implies that it, too, is symmetric. The non-zero elements of S^W are proportional to the desired matrix elements

$$S_{j,D}^W = c P_{jj} \langle j | [-i\mathcal{H}_W(0)] | D \rangle, \quad (\text{A3})$$

where $j = 1, 2$ runs over the $\pi\pi$ and $K\bar{K}$ channels, P is the square root of the phase space factor defined in Eq. (46), and c is a known real constant whose value will not be needed.

Unitarity of the complete S -matrix implies that the terms linear in the weak interaction satisfy

$$iS^W = S^{(0)}(iS^W)^\dagger S^{(0)}. \quad (\text{A4})$$

This implies that

$$iS_{j,D}^W = S_{jk}^s (iS_{D,k}^W)^* = S_{jk}^s (iS_{k,D}^W)^*, \quad (\text{A5})$$

where in the last step we have used the symmetry of S^W . Using the explicit form for the two-channel S -matrix¹⁰

$$S^s = R^{-1} \begin{pmatrix} e^{2i\delta_1} & 0 \\ 0 & e^{2i\delta_2} \end{pmatrix} R, \quad (\text{A6})$$

with

$$R = \begin{pmatrix} c_\epsilon & s_\epsilon \\ -s_\epsilon & c_\epsilon \end{pmatrix}, \quad (\text{A7})$$

we find

$$iR_{jk}S_{k,D}^W = e^{2i\delta_j} (iR_{jk}S_{k,D}^W)^*. \quad (\text{A8})$$

It follows that the phase of $iR_{jk}S_{k,D}^W$ is $e^{i\delta_j}$. This is the desired generalization of Watson's theorem to two channels. Thus the quantities

$$v_j = e^{-i\delta_j} \frac{1}{c} \sqrt{4\pi E^*} iR_{jk}S_{k,D}^W \quad (\text{A9})$$

are real. Using (A3) we can rewrite the v_j as in Eqs. (75) and (76).

If the weak interaction is not T invariant, then $S_{j,D}^W$ will contain some number of T-violating phases. Since we are working to linear order in the weak interaction, we can break up \mathcal{H}_W into parts each with a single T-violating phase and treat each separately. Each such part has an overall phase $e^{i\phi_T}$, the symmetry of the S -matrix is replaced by

$$S_{D,k}^W(\phi_T) = S_{k,D}^W(-\phi_T). \quad (\text{A10})$$

However, if we first pull out the overall phase by hand, then the symmetry of ΔS is restored, and Watson's theorem applies to the residue.

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¹⁰ For simplicity of presentation, we are here using $\delta_1 = \delta_\alpha$ and $\delta_2 = \delta_\beta$.

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