## **Final-State Interactions – A Lattice Perspective**

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## **Final-State Interactions – A Lattice Perspective**

# (Two-Pion States in Lattice QCD)

• In earlier talks at this workshop, we have heard about the determination of the LEC's of  $K \to \pi\pi$  decay amplitudes from the computation of  $K \to \pi$  and  $K \to 0$  matrix elements.

In this talk I will discuss the direct lattice evaluation of  $K \to \pi \pi$  matrix elements:

- the ultimate goal is to compute the amplitudes for physical kinematics;
- the intermediate aim is to facilitate the determination of the LECs at NLO in the chiral expansion.

• The study of the  $\Delta I = 1/2$  rule, and in particular the precise evaluation of  $\varepsilon'/\varepsilon$ , are extremely difficult projects.

Of the many theoretical and technical issues, I will focus largely on those related to having two-pion states  $\Rightarrow$  finite-volume effects which decrease as powers of the volume  $\Rightarrow$  evaluation of two-pion phase shifts from the spectrum.

### **Final-State Interactions – A Lattice Perspective**

• Finite-Volume Effects for  $\pi\pi$  states

C.-J.D.Lin, G.Martinelli, CTS & M.Testa Nucl.Phys.B619 (2001) 467 hep-lat/0111033

•  $K \to \pi \pi$  at NLO in  $\chi PT$ 

C.-J.D.Lin, G.Martinelli, E.Pallante, CTS, G.Villadoro Nucl.Phys.B650 (2003) 301; Phys.Lett.B553 (2003) 230; Phys.Lett.B581 (2004) 207

Some preliminary numerical results for ΔI = 3/2 transitions.
 P. Boucaud, V. Giménez, C.-J.D Lin, V. Lubicz, G. Martinelli, M. Papinutto & CTS (in preparation)

#### Lüscher Quantization Condition

M.Lüscher Nucl.Phys.**B354** (1991) 531

• In a cube of size  $L^3$  and under the assumption that only s-waves interact, two-pion states in the centre-of-mass frame satisfy the quantization condition

$$h(k,L) \equiv \frac{\phi(q) + \delta(k)}{\pi} = n$$
,

where:

\* n is a non-negative integer;

 $\ast~k$  is the relative momentum of the two-pion system with total center-of-mass energy E

$$k(E) = \sqrt{rac{E^2}{4} - m_\pi^2}$$
 and  $q \equiv rac{L}{2\pi}k$ ;

\*  $\delta(k)$  denotes the physical (infinite-volume) s-wave phase-shift; \* The function  $\phi$  is given by

$$\tan \phi(q) = -\frac{\pi^{\frac{3}{2}}q}{Z_{00}(1;q^2)} \quad \text{with} \quad Z_{00}(s;q^2) = \frac{1}{\sqrt{4\pi}} \sum_{n \in \mathbb{Z}^3} (n^2 - q^2)^{-s}$$

### Lüscher Quantization Condition – Comment 1

• In addition to the states satisfying the quantization condition there are *spurious* states satisfying the Schrödinger equation, e.g. consider

$$\phi(x) = e^{i\vec{p}_n \cdot \vec{x}} - e^{i\vec{p}'_n \cdot \vec{x}}$$

where

$$\vec{p}_n^2 = \vec{p}_n'^2 = \left(\frac{2\pi}{L}\right)^2 \vec{n}^2,$$

with the two momenta  $\vec{p_n}$  and  $\vec{p'_n}$  not related by a cubic transformation (e.g. (3,0,0) and (2,2,1) in units of  $2\pi/L$ ).

 $\phi(x)$  satisfies the Schrödinger equation but has no s-wave projection and all other angular momenta are non-interacting. The spurious states therefore do not contribute to  $K \to \pi\pi$  decays amplitudes or  $\pi\pi$  scattering amplitudes.

This is important in principle, since it allows the infinite-volume limit to be taken at fixed physics. LMST

### Lüscher Quantization Condition – Comment 2

• With cubic boundary conditions the energy eigenstates do not correspond to individual partial waves. However the quantization condition arises from the requirement that inside the volume V the s-wave component of the eigenfunctions is undistorted by the presence of the cubic boundary conditions:

$$\Psi_{E_n}^{V_{\text{s-wave}}}(r) = \frac{1}{\sqrt{c(E_n)}} \Psi_{E_n}^{\infty_{\text{s-wave}}}(r) \ .$$

where  $c(E_n)$  is a normalization constant.

$$\begin{aligned} \langle 0|\sigma(0)|\pi\pi;n\rangle_V &= \int_V d^3x \, S(r)\Psi_{E_n}^V(\vec{x}) = \int_V d^3x \, S(r)\Psi_{E_n}^{V_{\text{s-wave}}}(r) \\ &= \frac{1}{\sqrt{c(E_n)}} \int d^3x \, S(r)\Psi_{E_n}^{\infty_{\text{s-wave}}}(r) = \frac{1}{\sqrt{c(E_n)}} \langle 0|\sigma(0)|\pi\pi;E_n \rangle \end{aligned}$$

where I have assumed that S(r) (the coordinate representation of  $\sigma$ ) is localized within V.

Thus the relation between finite-volume and infinite-volume matrix elements of local operators is given by the relative normalization factors of the states.

#### Heuristic "Derivation" of the LL-Formula

Let  $\sigma(x)$  be a local scalar operator which can create two pions from the vacuum and consider the correlator (t > 0):

$$\int_{V} d^{3}x \langle 0|\sigma(x) \sigma(0)|0\rangle = V \sum_{n} |\langle 0|\sigma(0)|\pi\pi, n\rangle_{V}|^{2} e^{-E_{n}t}$$
$$\xrightarrow{V \to \infty} \int_{0}^{\infty} dE \rho_{V}(E) |\langle 0|\sigma(0)|\pi\pi, E\rangle_{V}|^{2} e^{-Et},$$

where the "density of states" is given by

$$\rho_V(E) = \frac{dn}{dE} = \frac{q\phi'(q) + k\delta'(k)}{4\pi k^2} E.$$

On the other hand, in infinite-volume we have

$$\int d^3x \left\langle 0 | \sigma(x) \, \sigma(0) \, | 0 \right\rangle = \frac{\pi}{2(2\pi)^3} \int \frac{dE}{E} e^{-Et} \left| \left\langle 0 | \sigma(0) \, | \pi\pi, E \right\rangle \right|^2 k(E) \, ,$$

where  $k(E) = \sqrt{E^2/4 - m_{\pi}^2}$ .

Comparing these two equations we establish the correspondence:

$$|\pi\pi, E\rangle \Leftrightarrow 4\pi \sqrt{\frac{VE\rho_V(E)}{k(E)}} |\pi\pi, E\rangle_V$$
.

Similar steps for single particle states at zero momentum give

$$|\vec{p}=0\rangle \Leftrightarrow \sqrt{2mV} \,|\vec{p}=0\rangle_V.$$

Combining the relations for single particle and two particle states, we obtain the LL relation for the physical amplitude:

$$|\langle \pi\pi, E = m_K | \mathcal{H}_W(0) | K \rangle|^2 = 8\pi V^2 \{ q\phi'(q) + k\delta'(k) \}_{k=k_\pi} \left( \frac{m_K}{k_\pi} \right)^3 |_V \langle \pi\pi, E | \mathcal{H}_W(0) | K \rangle_V |^2 \}$$

where  $k_{\pi} \equiv \sqrt{\frac{m_{K}^{2}}{4} - m_{\pi}^{2}}$ .

This derivation shows that the LL-factor is a property of the two-pion state, and does not require  $W_{2\pi} = m_K$ .

## Lüscher Quantization Condition – Comment 3

• So far we have considered the  $\pi\pi$  system at rest, but it would be very useful to know the quantization condition also in a moving frame.

• Rummukainen and Gottlieb (Nucl.Phys. **B450** (1995) 397) derive such a condition, based on Lüscher's derivation for  $\vec{p} = 0$ .

I am embarrassed to say that we do not understand the RG derivation and have been unable to derive the moving frame quantization condition using LMST techniques.

• Periodic boundary conditions in the moving frame  $\Rightarrow$  c.o.m. boundary conditions which involve both space and time coordinates.

- A key ingredient of the RG approach is the observation that outside of the interaction region the equations of motion imply that  $\phi_{\text{CoM}}(x^*)$  is independent of time ( $x^*$  is the relative coordinate in the CoM frame). - However, this is not true inside the interaction region, and so we cannot understand why t can be dropped in imposing the periodicity.

• Our embarrassment is compounded by the fact that: 1. RG perform numerical tests of their formulae in a toy theory. 2. The RG formula works at lowest non-trivial order of perturbation theory. (This is understandable since first order perturbation theory gives an energy shift of  $\langle \phi_0 | \mathcal{H}_1 | \phi_0 \rangle$ .) Quantization Condition and LL Factor in Perturbation Theory Consider the following correlation function in a  $\lambda \phi^4$  perturbation theory:

 $\langle 0 | \pi_{\vec{q}}(t_1) \pi_{-\vec{q}}(t_2) \sigma(0) | 0 \rangle$ , where  $\pi_{\vec{q}}(t) = \int d^3x \ \pi(\vec{x}, t) \exp(i\vec{q} \cdot \vec{x})$ ,



At this order, the correlator (for  $t_1 = t_2 = t$ ) is:

$$\mathcal{C}(W,t) = \mathcal{C}^{0}(W,t) \left\{ 1 - \lambda \left[ f(W) + \frac{z(1)}{4(2\pi)^{2}EL} + \frac{\nu}{L^{3}} \frac{3}{16E^{3}} + \frac{\nu}{L^{3}} \frac{1}{16E^{3}} \right] \right\} + \cdots$$

where  $E^2 = \vec{q}^2 + m^2$  and

$$z(s) = \sum_{\substack{\vec{l} \in Z^3 \\ |\vec{l}| \neq |\vec{n}|}} \frac{1}{(\vec{l}^2 - \vec{n}^2)^s} \quad \text{with} \quad \vec{q} = (2\pi/L) \, \vec{n}.$$

$$\mathcal{C}(W,t) = \mathcal{C}^{0}(W,t) \left\{ 1 - \lambda \left[ f(W) + \frac{z(1)}{4(2\pi)^{2}EL} + \frac{\nu}{L^{3}} \frac{3}{16E^{3}} + \frac{\nu}{L^{3}} \frac{1}{16E^{3}} \right] \right\} + \cdots$$

**1.**  $W = 2E + O(\lambda)$  is the energy of the state being considered and  $\nu$  is the corresponding degeneracy.

The energy shift due to the interactions in the finite volume is found to be

$$\Delta W = \frac{\lambda \nu}{4L^3 E^2}.$$

It appears as a linear term in t, and is absorbed into the exponential factor,

$$\exp(-2Et)(1-(\Delta W)t) \to \exp(-Wt).$$

 $\Delta W$  is precisely that obtained from the Lüscher quantization condition using the one-loop expression for  $\delta(k)$ .

$$\mathcal{C}(W,t) = \mathcal{C}^{0}(W,t) \left\{ 1 - \lambda \left[ f(W) + \frac{z(1)}{4(2\pi)^{2}EL} + \frac{\nu}{L^{3}} \frac{3}{16E^{3}} + \frac{\nu}{L^{3}} \frac{1}{16E^{3}} \right] \right\} + \cdots$$

2. In infinite volume the amplitude is proportional to  $1-\lambda f(W)$ . We have replaced a momentum sum by an integral.

**3.** & **4.** These two terms correspond to the expansion of the LL-factor, using the one-loop expression for  $\delta(k)$ .

5. This is the finite-volume correction to the two-pion sink, which is cancelled when we divide by the matrix element of the sink. This term depends, for example, whether we choose  $t_1 = t_2$  or  $t_1 \neq t_2$ .

## $\mathbf{K} \to \pi\pi$ Decays at NLO in the Chiral Expansion

- The evaluation of  $K \to \pi \pi$  decay amplitudes at physical kinematics will not be possible for some years yet, particularly in unquenched simulations. We will therefore continue to rely on  $\chi$ PT to estimate physical decay amplitudes from simulations at unphysical kinematics for some time.
- We have embarked on a major project to exploit  $\chi$ PT at NLO. The generic structure is of the form:

 $\langle \pi \pi | \mathcal{O}_W | K \rangle = \text{LO} * (1 + \text{Logs}) + \text{NLO counterterms.}$ 

The Logs are calculable in one-loop  $\chi$ PT. The idea is to use lattice computations of  $K \to \pi\pi$  matrix elements, for a range of masses and momenta, in order to

- determine the LO and NLO low-energy constants;
- use these to determine the physical decay amplitudes.
- We have determined the NLO expression for  $\Delta I = 3/2$  decays for both full and quenched QCD for general kinematics. (Full QCD calculation for  $\Delta I = 1/2$  decays being checked.)

Correlation Function in  $\chi PT$  (Full QCD) and Finite Volume



$$\langle 0|\pi_{-\vec{q}}(t_1)\pi_{\vec{q}}(t_2)\mathcal{O}_W(0)K_{\vec{0}}^{\dagger}(t_K)|0\rangle \simeq \frac{e^{-m_K|t_K|}}{2m_K}\frac{e^{-Et_2}}{2E}\frac{e^{-Et_1}}{2E}A_{\infty}(2E)[1+T]$$

with 
$$T = -(\Delta W)t_2 - \frac{C_{\text{sink}}}{E^3L^3} + \frac{c_1z(0)}{E^3L^3} + \frac{c_2z(1)}{EL} + \left(\frac{\partial A_{\infty}}{\partial E}\right)\frac{\Delta W}{2},$$
  
1. 2. 3. 4. 5.

Energy shift; 2. FV corrections from the two-pion sink;
 & 4. LL Factor for the Matrix Element; 5. Shifts the energy in A.

### Quenched Amplitude in Finite Volume

$$\langle 0|\pi_{\vec{q}}(t_1)\pi_{-\vec{q}}(t_2)\sigma(0)|0\rangle = \frac{e^{-E_q t_1}}{2E_q} \frac{e^{-E_q t_2}}{2E_q} \left(\frac{-8}{f^2}\right) \left[1 + A_{\infty}^{(1)} + T\right]$$

$$f^{2}T = a_{1}\frac{\nu}{E^{2}L^{3}}t_{2} + a_{2}\frac{\nu}{EL^{3}}t_{2}^{2} + a_{3}\frac{\nu}{L^{3}}t_{2}^{3} + \frac{\nu(b_{1}+b_{2}t_{1}+b_{3}t_{1}^{2})}{E^{3}L^{3}} + c_{1}\frac{z(0)}{E^{3}L^{3}} + c_{2}\frac{z(1)}{EL} + c_{3}z(2)EL + c_{4}z(3)E^{3}L^{3} - \frac{5.6}{6.5} - \frac{5.6}{7.5} - \frac{5.6}{7.$$

- Infinite volume phase-shift depends on the operator.
- There are non-standard FV "corrections" (7. & 8.).

### What is the origin of these sick features?

### Hairpin Diagrams and Double Poles

As an example consider the following  $\Delta I = 1/2$  contribution to decay  $\bar{K}^0 \to \pi^+ \pi^-$  in quenched QCD:



• Qualitatively the  $\eta'$  propagator is rewritten as the first two terms of the pion propagator.

Double Pole  $\Rightarrow$  more singular long-distance behaviour.

• At one-loop order in the chiral expansion there are no such contributions to  $\Delta I = 3/2$  transitions.

### Lack of Unitarity in Quenched QCD

In full QCD we have the following contribution to the  $\Delta I = 1/2$  decay  $\bar{K}^0 \to \pi^+ \pi^-$ :



• In the quenched theory this contribution is absent. This is achieved, e.g. by introducing ghost-quarks (with the opposite statistics) to cancel the effect.

Internal particles are not the same as the external ones  $\Rightarrow$  FSI depend on the operator.

• At one-loop  $\chi$ PT this effect is not present for  $\Delta I=3/2$  decays.

• These effects, due to lack of unitarity, are also present for partially quenched QCD, when allowed real intermediate states are not the same as the external ones.

Thus for example for two flavours of sea quark, the sicknesses of the quenched theory reappear when  $W > 2m_K$ .

• An amusing aside is that even in full QCD, but with exact SU(3) flavour symmetry, the extraction of two-pion matrix elements is subtle:

$$|1\rangle = \frac{1}{2}\sqrt{\frac{3}{2}}|\pi\pi\rangle + \frac{1}{\sqrt{2}}|KK\rangle + \frac{1}{2\sqrt{2}}|\eta\eta\rangle$$
$$|8\rangle = -\sqrt{\frac{3}{5}}|\pi\pi\rangle + \frac{1}{\sqrt{5}}|KK\rangle + \frac{1}{\sqrt{5}}|\eta\eta\rangle$$
$$|27\rangle = \frac{1}{\sqrt{40}}|\pi\pi\rangle - \sqrt{\frac{3}{10}}|KK\rangle + \sqrt{\frac{27}{40}}|\eta\eta\rangle$$

Thus, for example, we would need a suitable combination of  $\langle 1, 8, 27 | Q_6 | K^0 \rangle$  amplitudes to obtain the required  $\langle \pi \pi | | Q_6 | K^0 \rangle$  matrix element.(This requires the evaluation of  $K^0 - Q_6 - (\phi \phi)_i$  and  $(\phi \phi)_i - (\phi \phi)_i$  correlators.)

In a single finite volume the three two-meson states  $|1\rangle$ ,  $|8\rangle$  and  $|27\rangle$  acquire different energies. Thus, in principle, one needs to tune the volumes for each of the representations to ensure that the energy is the same in the three cases.

An exploratory study of matrix elements of  $\Delta I = 3/2 \ K \rightarrow \pi \pi$ decays at next-to-leading order in the chiral expansion

• We have performed a quenched study of  $\Delta I = 3/2 \ K \rightarrow \pi \pi$  matrix elements:

340+480 configurations on a  $24^3 \times 64$  lattice,

 $a^{-1} = 1.98(6)$  GeV, Improved Wilson Action,

SPQR Kinematics (kaon and one pion a rest, second pion with momentum zero or  $(2\pi/L, 0, 0)$ ).

• The matrix elements can be determined successfully. Nevertheless, on the basis of this simulation and our theoretical studies we expect to do much better in a second generation simulation.



We evaluate correlation functions of the form:

$$G_{4\pi}(t,\vec{p}) = \frac{1}{2} \left( \left\langle P_{\pi^{+}}(t,\vec{p}) P_{\pi^{0}}(t,\vec{0}) \phi_{\pi^{+}}^{\dagger}(\vec{0},0) \phi_{\pi^{0}}^{\dagger}(\vec{0},0) \right\rangle + \left\langle P_{\pi^{+}}(t,\vec{0}) P_{\pi^{0}}(t,\vec{p}) \phi_{\pi^{+}}^{\dagger}(\vec{0},0) \phi_{\pi^{0}}^{\dagger}(\vec{0},0) \right\rangle \right)$$

and  $C_{PP}(t,\vec{p}) = \langle 0|P_P(t,\vec{p})\phi_P^{\dagger}(\vec{0},0)|0\rangle$ , where  $P_P(t,\vec{p}) \equiv \int d^3x \ e^{-i\vec{p}\cdot\vec{x}}\phi_P(\vec{x},t)$ .

For small energy shifts

$$R_{4\pi}(t;\vec{p}) \equiv \frac{G_{4\pi}(t;\vec{p})}{C_{\pi}(t,\vec{p})C_{\pi}(t,\vec{0})} \propto \exp(-\Delta W t) = 1 - \Delta W t \,.$$

Slope of  $R_{4\pi} \Rightarrow$  Energy Shift.



• Only diagrams D & C contribute to I = 2 correlators.



$M_{\pi}$	0.4438(7)	0.3590(8)	0.2557(13)
$\Delta W_{\vec{p}=0}$	0.0054(6)(7)	0.0062(7)(7)	0.0066(9)(7)
$\Delta W_{\vec{p}=\frac{2\pi}{L}}$	0.0086(8)(10)	0.0109(11)(15)	0.0152(27)(15)
$\Delta W_L^{-L}$	0.0064(3)	0.0072(3)	0.0083(5)
$\Delta W_{BG}$	0.0052(2)	0.0060(2)	0.0071(3)

• In the range of masses which we have, (0.5, 1.2 - 1.5) GeV, (quenched)  $\chi$ PT gives poor fits (even if we impose an upper cut-off of 0.8 GeV).

 $\bullet$  The data is beautifully described by polynomials, i.e. by NLO  $\chi \rm PT$  without the logarithms.



• In order to obtain reliable results we must perform unquenched simulations at smaller masses in order to obtain data which follows NLO  $\chi$ PT.

In the meantime we estimate the matrix elements by using the *Centaur* procedure of smoothly matching our lattice data (the *horse*) to  $\chi$ PT (the *man*) at some matching point.

• For the EWP operators the results are very stable. For  $O_4$  (for which the LO result is  $O(p^2)$ ) they are less so (although the LO LEC is well determined).

Results to Follow.

### **Prospects and Conclusions**

• Reliable calculations of  $\Delta I = 3/2 \ K \rightarrow \pi \pi$  amplitudes are possible, and will be performed before Eduardo retires.

• We understand how to calculate physical  $K \to \pi \pi$  amplitudes in principle. The use of NLO  $\chi$ PT will be a useful tool in the next few years.

The chiral expansion has been calculated for general kinematics to NLO for  $\Delta I = 3/2$  transitions and is being checked for  $\Delta I = 1/2$  ones.

• We are currently learning how to calculate the R and V diagrams most effectively:



• It would be very useful to have a theoretical control of the finite-volume effects in a moving frame.

• Quenched calculations of I = 0 correlation functions are explicitly unphysical, and partially quenched ones are *partially* unphysical.

It is time to a bandon quenched calculations in general, and particularly of I = 0 correlation functions.