Lattice QCD and the Timelike Pion Form Factor

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We present a formula that allows one to calculate the pion form factor in the timelike region $2m_\pi \leq \sqrt{s} \leq 4m_\pi$ in lattice QCD. The form factor quantifies the contribution of two-pion states to the vacuum polarization. It must be known very accurately in order to reduce the theoretical uncertainty on the anomalous magnetic moment of the muon. At the same time, the formula constitutes a rare example where, in a restricted kinematic regime, the spectral function of a conserved current can be determined from Euclidean observables without an explicit analytic continuation.

I. INTRODUCTION

The ab initio calculation of hadron properties in lattice QCD is a mature and ongoing research activity. For a compilation of results for some quantities of high phenomenological impact see Ref. [1]. One important aspect of lattice QCD is that it is formulated in Euclidean space. Therefore the form factors are necessarily extracted for momentum transfers in the spacelike region, $q^2 \equiv q_0^2 - q^2 = -Q^2 < 0$. At first sight, it thus seems that a form factor in the timelike region, or more generally any quantity which involves the notion of ‘real time’, is only accessible via analytic continuation. The latter typically involves solving a Fredholm equation of the first kind such as Eq. (9), which represents a numerically ill-posed problem 2.

The goal of this letter is twofold. First, to provide an example where, in a certain kinematic regime, a spectral function (to be defined shortly) can be extracted from Euclidean field theory without an explicit analytic continuation. And secondly, to lay the ground for future calculations of the pion form factor in the timelike region, which may impact the theoretical determination of the anomalous magnetic moment of the muon. Given the high likelihood of a new ($g - 2)_\mu$ experiment at Fermilab [3], this application is particularly timely.

For the electromagnetic current $j_{\mu}^{em} = \frac{2}{3} u \gamma_\mu u - \frac{1}{3} d \gamma_\mu d + \ldots$ the spectral function is defined as

$$\rho_{\mu\nu}(k) \equiv \frac{1}{2\pi} \int d^4 x e^{i k \cdot x} \langle 0 | [j_{\mu}^{em}(x), j_{\nu}^{em}(0)] | 0 \rangle.$$  \hfill (1)

Due to current conservation and Lorentz invariance, the tensor structure of $\rho_{\mu\nu}$ is

$$\rho_{\mu\nu}(k) = - (g_{\mu\nu} k^2 - k_\mu k_\nu) \cdot \rho(k^2).$$ \hfill (2)

The spectral density $\rho$ is non-negative. The leading hadronic contribution to the vacuum polarization $e^2 \Pi(Q^2)$ in the spacelike domain can be expressed through it via a once-subtracted dispersion relation,

$$\Pi(0) - \Pi(Q^2) = Q^2 \int_0^\infty ds \frac{\rho(s)}{s(s + Q^2)}.$$ \hfill (3)

The function $\Pi(Q^2)$ can be calculated in lattice QCD [4-7]. On the other hand, $\rho(s)$ is related to experimental observables,

$$\rho(s) = \frac{R(s)}{12\pi^2}, \quad R(s) \equiv \frac{\sigma(e^+ e^- \to \text{hadrons})}{4\pi\alpha(s)^2/(3s)}.$$ \hfill (4)

The denominator is the treelevel cross-section $e^+ e^- \to \mu^+ \mu^-$ in the limit $s \gg m_\mu^2$, and we have neglected QED corrections. At low energies, the spectral density is given by the pion form factor defined in [12-18].

$$\rho(s) = \frac{1}{18\pi^2} \left(1 - \frac{4m_\pi^2}{s}\right)^2 |F_\pi(\sqrt{s})|^2, \quad |F_\pi(0)| = 1.$$ \hfill (5)

The relation holds for $2m_\pi \leq \sqrt{s} \leq 3m_\pi$, and even up to $4m_\pi$ if the electromagnetic current is replaced by the isospin current in the definition of $\rho(s)$.

In infinite volume, the spectral density is a continuous function above the two-particle threshold. In finite volume, where simulations are carried out, it is a collection of delta functions. What is needed is an explicit formula that relates the energy and matrix element of one individual state living on the 3d torus to the infinite-volume spectral density at the same energy. In this letter we derive the formula

$$|F_\pi(E)|^2 = \left(q^0 \phi(q) + k \frac{\partial \delta_1(k)}{\partial k} \right)^2 \frac{3\pi E^2}{2k^5} |A_\psi|^2.$$ \hfill (6)

Here $E$ equals the invariant mass of the two pions, $k$ is related to $E$ via Eq. (4), $\delta_1$ is the scattering phase shift in the unit isospin, $p$-wave channel and $A_\psi$ is a vector-current matrix element between the vacuum and a two-pion state $|\psi^p_\pi\rangle$ of energy $E$ on the torus, see Eq. (7). Finally, $q \equiv \frac{2\pi i}{a}$ and $\phi$ is a known kinematic function [6]. The scattering phase $\delta_1(k)$ can be extracted (see [11] and Refs. therein) from the finite-volume spectrum using the Lüscher formula [12, 13], Eq. (7).

The derivation of Eq. (6) is closely related to work by Lellouch-Lüscher [13] on the matrix element determining the $K \to \pi\pi$ decay rate. Eq. [5,6] show that this formula, remarkably, allows one to extract a spectral function from Euclidean field theory without an explicit analytic continuation.
II. PRELIMINARIES

We will assume here that isospin is an exact symmetry of QCD, and focus on the vector isovector channel
\[ I = 1, \quad J^{PC} = 1^{-}. \]  

Both in experiment and in the Euclidean theory, the symmetry of the final state can be selected. Therefore, in spite of the physical photon not having definite isospin quantum numbers, we will consider the case of a gauge boson coupling to the isospin current
\[ j_\mu^a = \bar{\psi} i \gamma_\mu T^a \psi, \quad \psi = \left( \begin{array}{c} u \\ d \end{array} \right). \]  

In infinite volume, and with quark masses set to their physical values, the states in the symmetry channel are necessarily two-pion states for center-of-mass energies
\[ 2m_\pi \leq E \leq 4m_\pi. \]  

We are thus led to consider pion scattering in this energy range. First, the normalization of single-pion states is
\[ (a|b) = \delta_{ab}(2\pi)^3 2E_a \delta(k-k'). \]  

The \( T_1 \) matrix describing the scattering of two pions is defined in full generality in [9, Sec. 2.1]. It carries an isospin index \( I = 0, 1, 2 \); here we are interested in the \( I = 1 \) channel. The \( T_1 \) matrix can be expanded in partial waves with amplitudes \( t_\ell \), with corresponding phase shifts \( \delta_\ell \). We restrict ourselves to the \( \ell = 1 \) partial wave in the elastic regime,
\[ T_1 = 48\pi E_{\pi\pi} t_{11} \cos \theta, \quad t_{11} = \frac{\epsilon^{2i\delta_{11}} - 1}{2ik_\pi}. \]  

From now on the phase shift will simply be written \( \delta_1 \). When the pions couple to the photon, they can be produced for example in the reaction \( e^+e^- \to \gamma \to \pi\pi \).

With \( (\pi_\rho \pi_\rho) = \frac{2k}{\sqrt{N}} (\pi_\rho \pi_\rho) \), the pion form factor in the timelike region is defined as [14]
\[ \langle 0| j^a |(\pi_\rho \pi_\rho)^b \rangle, \text{in} \rangle = -\langle \langle \pi_\rho \pi_\rho \rangle, \text{out} \rangle \langle j^a | 0 \rangle = \delta^{ab} \frac{i}{2 \Gamma} (p - p) F_\pi(E_{\pi\pi}). \]  

The two-pion states on a three-dimensional torus of dimensions \( L \times L \times L \) at vanishing total momentum have been studied in detail in [4]. The vector states \( \ell = 1 \) are found exclusively in the \( T_1 \) irreducible representation of the cubic group. Their norm will be taken to be unity. We denote by \( E_{\pi\pi} \) the energy of one such state. The effective momentum of the pion \( k_\pi \) is then defined by the equation
\[ E_{\pi\pi} = 2\sqrt{m_\pi^2 + k_\pi^2}. \]  

The function \( \phi(q) \) is defined by \( \tan \phi(q) = \frac{q^{3/2}}{Z_{00}(1,q^2)} \), where \( Z_{00}(1,q^2) \) is the analytic continuation in \( s \) of \( Z_{00}(s,q^2) = \frac{1}{4\pi} \sum_{n \in Z^3} \frac{1}{(n^2 + q^2)^2} \).

III. QCD COUPLED TO \( SU(2)_l \) GAUGE BOSONS IN THE BROKEN PHASE

The theory we consider is QCD with at least two degenerate light flavors of quarks \( u \) and \( d \). The other flavors are assumed to be sufficiently massive that the only unit-isospin states in the interval are the two-pion states. This is realized for physical values of the quark masses.

We now wish to establish Eq. (13) in the regime where the gaps between finite-volume energy eigenstates are substantial, which is the situation that can realistically be achieved in Monte-Carlo simulations. The idea is to couple the quarks infinitesimally (the coupling will be denoted by \( e \)) to an external vector particle with mass in the range [13]. On one hand, when it is degenerate with a two-pion energy eigenstate in the box, a level splitting of order \( e \) occurs; on the other hand, in infinite volume the resonant production of the vector particle in pion scattering leads to an \( O(e) \) change in the phase shift. The phase shift and the energy levels in the box must be in correspondence through the Lüscher formula [14] both before and after switching on the coupling \( e \). Eq. (13) follows from the difference of these relations. The proof is thus almost identical to the proof of the Lellouch-Lüscher formula for the kaon decay [13]. The only qualitative differences are that we are in a different symmetry channel and, more importantly, that we invoke an external particle. A similar formula for a matrix element involving a two-particle state was derived in [14], in the large-volume regime where individual states are too narrowly spaced to be individually resolved.

A concrete model for the massive vector boson is not required in the proof, but it may be reassuring for the validity of the argument that the situation sketched above can be realized within a renormalizable field theory. A specific realization, then, involves gauging the isospin symmetry (this was, incidentally, the original motivation of Yang and Mills [16] to introduce non-Abelian gauge theories). There are then three gauge bosons of the group \( SU(2)_l \). Since we want them to be massive, we assume that the gauge group is spontaneously broken by a Higgs mechanism at a scale well above \( \Lambda_{\text{QCD}} \), the scalar field being in the fundamental representation of \( SU(2)_l \). The three gauge bosons \( W^a \) then form a degenerate triplet of mass \( M \), which we assume to be in the range [13]. They have the same quantum numbers as the \( \rho \) meson and couple to the isospin current.
A. Two-pion energy levels in finite volume

We start with the system in finite volume and study the effect of the massive gauge bosons on the low-lying spectrum, which consists of two-pion states. The gauge boson field operator reads

$$A^\mu(x) = \sum_k \sum_{\sigma=1}^3 \frac{e^\mu(k)}{2E_kL^2} (a^\mu_{k,\sigma} e^{ikx} + a^\dagger_{k,\sigma} e^{-ikx}),$$

(15)

with $[a^\mu_{k,\sigma}, a^\dagger_{k',\sigma'}] = \delta^{\sigma\sigma'} \delta_{kk'}$ and the polarization vectors $e^\mu_\sigma$ are such that at $k = 0$, $e^\mu_0 = 0$ and $e^\mu_\sigma = \delta_{\sigma j}$. The coupling to the massive gauge bosons is treated as a perturbation, with

$$H_{\text{int}} = +e \int j^{\mu}(x) A^\mu(x).$$

(16)

The box size $L$ is now chosen such that the energy eigenvalue of a unit-norm, non-degenerate state $|\psi^a_\sigma\rangle$ of the two-pion system overall at rest in the box satisfies $E^{z\pm}_{\pi\pi} = M$ when $e$ is set to zero. Upon switching on the SU(2)$_L$ gauge interaction, we apply degenerate perturbation theory of quantum mechanics. The two-pion state mix maximally with the massive gauge boson state $|W^\mu\sigma\rangle \equiv q_{0\sigma}|0\rangle$, since they are initially degenerate, and the splitting between the two resulting energy levels is given by the off-diagonal matrix element,

$$E^{z\pm}_{\pi\pi} = M \pm |A|$$

(17)

with

$$\langle \psi^a_\sigma | H_{\text{int}} | W^b_{\sigma'} \rangle = \delta^{ab} \delta_{\sigma\sigma'} A^\mu \frac{-e}{\sqrt{2M}} A^\mu \delta^{ab} \delta_{\sigma\sigma'},$$

(18)

$$L^{3/2} \langle \psi^a_\sigma | W^b_{\sigma'}(x)|0\rangle = \delta^{ab} \delta_{\sigma\sigma'} A^\mu \frac{-e}{\sqrt{2M}} A^\mu \delta^{ab} \delta_{\sigma\sigma'} A^\mu.$$ 

(19)

B. Pion-pion scattering in infinite volume

The coupling of quarks to the massive gauge bosons affects their scattering amplitude. At ordinary energies, the effect is $O(e^2)$. However, at the energy $E_{\pi\pi}$ the effect is enhanced to $O(e)$, due to the resonant production of a massive gauge boson, whose propagator reads

$$\frac{i\delta^{ab}}{p^2 - M^2 + i\epsilon} \left( P_{\mu} P_{\nu} \frac{1}{M^2} - g_{\mu\nu} \right).$$

(20)

The change of the scattering amplitude due to this process then reads, at the energy $E_{\pi\pi}$ and with center-of-mass frame kinematics,

$$\Delta T_1 \left( (\pi^- \pi^-)^a \rightarrow W \rightarrow (\pi^+ \pi^-)^b \right)$$

(21)

$$= ([\pi^+ \pi^-]^b, \text{out} |j^d|^0) \cdot \frac{e^{2\delta^{ab}}}{q^2 - M^2} \cdot |0| j^d |(\pi^+ \pi^-)^a, \text{in} \rangle,$$

where $q^2 - M^2 = \pm 2M|A| + O(A^2)$. Using the definition of the pion form factor in the timelike region $\langle 2 \rangle$ and the phase $F_{\pi} = |F_{\pi}| e^{i\delta_1}$ due to Watson's theorem, we obtain

$$\Delta T_1 = \frac{e^{2\delta^{ab}}}{M|A|} F_{\pi}(E_{\pi\pi} = M)^2 4k^2 \cos \theta e^{2i\delta_1}.$$ 

(22)

Next we translate this into a change in the phase shift via Eq. $\langle 1 \rangle$.

$$\Delta \delta_1 = \frac{e^2}{12\pi M|A|} |F_{\pi}|^2 \frac{k^2}{E_{\pi\pi}}.$$ 

(23)

C. Connection between the energy levels in finite-volume and the scattering phase shift

We now go back to the finite volume system where $L$ is tuned so that $E_{\pi\pi} = M$. Upon switching on the perturbation $\langle 16 \rangle$, this degenerate energy level in the box splits, corresponding to $k \rightarrow k + \Delta k$, where in view of Eq. $\langle 13 \rangle$–$\langle 17 \rangle$, $\Delta k = \pm A \frac{E_{\pi\pi}}{M}$. The phase shift that corresponds to the perturbed state by L"uscher's formula $\langle 14 \rangle$ differs from the phase shift corresponding to the unperturbed state by

$$\delta_1(k) \rightarrow \delta_1(k) + \frac{\partial \delta_1(k)}{\partial k} \Delta k + \Delta \delta_1(k).$$

(24)

In Eq. $\langle 14 \rangle$, this variation must be compensated by the change in the second term of the LHS,

$$\phi(q) \rightarrow \phi(q) + \phi'(q) \Delta q, \quad \Delta q = \frac{\Delta k}{k}.$$ 

(25)

Altogether, we then obtain the condition

$$\Delta \delta_1(k) = -\left( \phi'(q) + \kappa \frac{\partial \delta_1(k)}{\partial k} \right) \frac{\Delta k}{k}.$$ 

(26)

Inserting expression $\langle 28 \rangle$ for the change in the phase shift due to the resonant scattering, one then obtains Eq. $\langle 6 \rangle$.

D. Consistency check in the absence of pion-pion interactions

In the case where the two pions do not interact, the $n$th two-pion energy level $E_{\pi\pi}^n$ passes through $M$ for $\langle 13 \rangle$

$$L = \frac{2\pi}{k_{\pi}} \sqrt{n}, \quad 1 \leq n \leq 6,$$

(27)

$k_{\pi}$ being related to $E_{\pi\pi}$ by Eq. $\langle 13 \rangle$. From the definition of $\phi$, one sees that for $q^2 \rightarrow n$ an integer,

$$q \phi'(q) = (2\pi)^2 \frac{q^3}{\nu_n},$$

(28)

where $\nu_n$ is the number of vectors $z \in \mathbb{Z}^3$ with $z^2 = n$. The result $\langle 4 \rangle$ then becomes for non-interacting pions

$$|F_{\pi}(E_{\pi\pi} = M)|^2 = \frac{3}{4\nu_n} \frac{M^2 L^3}{k_{\pi}^2} |A|.$$ 

(29)
Finite-volume matrix element

One can check this last equation directly. Take for instance as a two-pion state on the torus $|\psi_p^a\rangle$ given by

$$|\psi_p^a\rangle = \frac{\epsilon^{abc}}{\sqrt{2}} a_p^{b\dagger} a_{-p}^{c\dagger} |0\rangle,$$

with $p = \hat{p} \hat{c}_3$ and $a_p^{b\dagger}$ a pion creation operator. Thus from the difference in normalization of the finite and infinite-volume states (Eq. 30 and 10) one predicts

$$8k_p^2 |F_{\pi\pi}|^2 = M^2 L^3 |A_{\psi}|^2,$$

which matches 29 for $\nu_n = 6$. This is precisely the multiplicity $\nu_n$ of $n = 1$ and 4 for which the only vectors $z$ are $(\sqrt{n}, 0, 0)$ and images thereof under cubic symmetries.

IV. ILLUSTRATION

Here we apply Eq. (9) to infer the dependence of the matrix element $A_{\psi}$ on $L$ from experimental scattering data. The scattering phase $\delta_1(k)$ is parametrized by

$$\frac{k^3}{E_{\pi\pi}} \cot \delta_1(k) = \frac{4k_p^4}{m_{\rho}^2} \left(1 - \frac{k^2}{k_p^2}\right),$$

with $k_p \equiv \sqrt{m_{\rho}^2 - 4m_{\pi}^2}$. In this effective range formula, the scattering phase is thus determined by the mass and width of the $\rho$ meson. Secondly, we extract the pion form factor from experimental data compiled by the PDG 17. At low energies the data is well described by

$$|F_{\pi}(E_{\pi\pi})|^2 = v_0 + v_1 \left(\left(E_{\pi\pi}/m_{\pi}\right)^2 - v_2^2 + v_3^2\right)^{-1},$$

where the fit parameters for the interval $2.0 m_{\pi} \leq E_{\pi\pi} \leq 4.4 m_{\pi}$ take the values $v_0 = 0.6473$, $v_1 = 10.59$, $v_3 = 0.1271$, and the $\chi^2/d.o.f.$ amounts to 1.2. We did not fit $v_2$, but set it to the value $m_{\rho}/m_{\pi} = 5.553$.

Using formula Eq. (9), we can predict the magnitude of the finite-volume matrix element $A_{\psi}$ up to the inelastic threshold in the $I = 1$ channel $(4m_{\pi})$. The result of this exercise is displayed in Fig. 1, along with the finite-volume matrix element one would expect if there were no interactions between the pions. As already discussed in 9, the size of the matrix element $|A_{\psi}|^2$ is of order $L^{-3}$ in the absence of interactions between the pions, but it would be strongly enhanced in the vicinity of a resonance.

V. CONCLUSION

We have derived a formula which connects Euclidean observables with the vector current spectral function in the elastic regime. Such a relation could have interesting applications in other systems, such as cold Fermi gases 18. Also, the idea to invoke an external particle weakly coupled to QCD is likely to lead to other important relations. Apart from its theoretical appeal, Eq. (9) provides a more direct way to compare lattice calculations with experimental determinations of $\rho(\sigma)$ than the dispersion relation 3. To complement the low-energy experiments constraining the leading hadronic contribution to $(g - 2)_\mu$, lattice simulations would have to reach very low pion momenta. For this purpose 19, 21, as well as to obtain the factor $\partial \delta_1(k)/\partial k$ 22, twisted boundary conditions could prove very useful.

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