We calculate the pion transition form factor $F_{\pi^0 \gamma^* \gamma^*}(q_1^2, q_2^2)$, which describe the interaction of an on-shell pion with two off-shell photons, using lattice QCD simulations with two degenerate flavors of dynamical quarks. This form factor is the main ingredient in the calculation of the pion-pole contribution to hadronic light-by-light scattering in the muon $g-2$, $a_{\mu}^{\text{HLL}}$. We focus our study on the spacelike region with photon virtualities up to $1.5$ GeV$^2$, not yet measured experimentally. Several lattice spacings and pion masses are used to extrapolate the results to the physical point and a comparison with different phenomenological models is performed. Finally, we use our extrapolated form factor to provide a lattice determination of $a_{\mu}^{\text{HLL}}$. 

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1. Introduction

The anomalous magnetic moment of the muon provides one of the most precise tests of the Standard Model of particle physics [1, 2] and a persistent discrepancy of about 3 – 4 standard deviations [3] exists between experiment and theory. In the near future, the experimental error is expected to be reduced by a factor four [4]. The theoretical error is now dominated by hadronic contributions: the hadronic vacuum polarization (HVP) and hadronic light-by-light scattering (HLbL) and, for the latter, no reliable estimate exists yet and systematic errors are difficult to estimate. However, recently a dispersive approach was proposed [5] which relates the numerically dominant pseudoscalar-pole contribution, and the pion-loop in HLbL with on-shell intermediate pseudoscalar states to measurable form factors and cross-sections with off-shell photons: \( \gamma^* \gamma^* \rightarrow \pi^0, \eta, \eta' \) and \( \gamma' \gamma' \rightarrow \pi^+ \pi^-, \pi^0 \pi^0 \). Within this framework, the pion-pole contribution is obtained by integrating some weight functions times the product of a single-virtual and a double-virtual transition form factors for spacelike momenta \([1]\). In particular, the weight functions turn out to be peaked at low momenta such that the main contribution to \( d_{\text{HLbL}}^{\pi^0,\gamma\gamma} \) arises from photon virtualities below 1 GeV\(^2\) [6], a kinematical range accessible on the lattice. From the experimental point of view, only the single-virtual form factor for the pion \( \mathcal{F}_{\pi^0,\gamma\gamma}(Q^2, 0) \) has been measured \([7]\) in the spacelike region \( Q^2 \in [0.5, 40] \) GeV\(^2\). From the theoretical point of view, the form factor is constrained by the Adler-Bell-Jackiw (ABJ) anomaly in the chiral limit such that \( \mathcal{F}_{\pi^0,\gamma\gamma}(0, 0) = 1/(4\pi^2 F_\pi) \) [8]. The single-virtual form factor has been computed in the framework of factorization in QCD (operator-product expansion (OPE) on the light-cone) and one finds the Brodsky-Lepage behavior \([9]\)

\[
\mathcal{F}_{\pi^0,\gamma\gamma}(Q^2, 0) \xrightarrow[Q^2 \to \infty]{} 2F_\pi/Q^2. \tag{1.1}
\]

Finally, the double-virtual form factor where both momenta become simultaneously large has been computed using the OPE at short distances. In the chiral limit the result reads \([10, 11]\)

\[
\mathcal{F}_{\pi^0,\gamma\gamma}(Q^2, -Q^2) \xrightarrow[Q^2 \to \infty]{} 2F_\pi/(3Q^2). \tag{1.2}
\]

Therefore, the double-virtual form factor in the kinematical range of interest \([0 – 1]\) GeV\(^2\) for the computation of the HLbL contribution to the muon \( g – 2 \) is still unknown and the available estimates rely on phenomenological models \([1, 12]\). Previous lattice studies \([13]\) < on the decay \( \pi^0 \to \gamma\gamma \) (form factor at very low momenta). More details on this work can be found in \([14]\).

2. Methodology

In Minkowski spacetime, the form factor of interest is defined via the following matrix element

\[
M_{\mu\nu}(p, q_1) = i \int d^4x e^{iq_1x} \langle \Omega | T \{ J_\mu(x) J_\nu(0) \} | \pi^0(p) \rangle = \epsilon_{\mu\nu\alpha\beta} q_1^\alpha q_2^\beta \mathcal{F}_{\pi^0,\gamma\gamma}(q_1^2, q_2^2), \tag{2.1}
\]

where \( q_1 \) and \( q_2 \) are the photon momenta and \( p = q_1 + q_2 \) is the on-shell pion momentum. \( J_\mu = \Sigma_f Q_f \bar{\psi}_f \gamma_\mu \psi_f \) is the hadronic component of the electromagnetic current and we use the relativistic normalization of states \( \langle \pi^0(p) | \pi^0(p') \rangle = (2\pi)^3 2E_\pi(p) \delta^{(3)}(p - p') \). To compute the form factor on the lattice, we follow the method introduced in \([15]\). Keeping \( q_{1,2}^2 < M_\psi^2 = \min(M_\psi^2, 4m_\pi^2) \), one can show \([16]\) that the matrix element in Euclidean spacetime is

\[
M_{\mu\nu} = (i\gamma^0)M_{\mu\nu}^E, \quad M_{\mu\nu}^E \equiv - \int d\tau e^{i\omega \tau} \int d^3z e^{-i\vec{q}z} \langle 0 | T \{ J_\mu(z, \tau) J_\nu(0) \} | \pi(p) \rangle, \tag{2.2}
\]
where $\omega_t$ is a real free parameter such that $q_t = (\omega_t, \vec{q}_t)$ and $n_0$ denotes the number of temporal indices carried by the two vector currents. Therefore, one is led to consider the following three-point correlation function on the lattice

$$C^{(3)}_{\mu\nu}(\tau, t_{\pi}) = a^6 \sum_{\vec{x}, \vec{z}} \langle T \left\{ J_\mu(\vec{z}, t_{\pi}) J_\nu(\vec{0}, t_f) P^I(\vec{x}, t_0) \right\} \rangle e^{i\vec{q}_t \cdot \vec{z}}, \quad (2.3)$$

where $\tau = t_i - t_f$ is the time separation between the two vector currents and $t_{\pi} = \min(t_f - t_0, t_i - t_0)$. The matrix element with on-shell pion is obtained by considering the large $t_{\pi}$ limit. By defining

$$A_{\mu\nu}(\tau) = \lim_{t_{\pi} \to +\infty} C^{(3)}_{\mu\nu}(\tau, t_{\pi}) e^{E_{\pi} t_{\pi}}, \quad \tilde{A}_{\mu\nu}(\tau) = \begin{cases} A_{\mu\nu}(\tau) & \tau > 0 \\ A_{\mu\nu}(\tau) e^{-E_{\pi} \tau} & \tau < 0 \end{cases}, \quad (2.4)$$

and using Eq. (2.2), $M_{\mu\nu}$ can be obtained via

$$M^{E}_{\mu\nu} = \frac{2E_{\pi}}{Z_{\pi}} \left( \int_{-\infty}^{0} d\tau e^{i\omega_{\pi} \tau} A_{\mu\nu}(\tau) e^{-E_{\pi} \tau} + \int_{0}^{\infty} d\tau e^{i\omega_{\pi} \tau} A_{\mu\nu}(\tau) \right) = \frac{2E_{\pi}}{Z_{\pi}} \int_{-\infty}^{\infty} d\tau e^{i\omega_{\pi} \tau} \tilde{A}_{\mu\nu}(\tau), \quad (2.5)$$

where the overlap factor $Z_{\pi}$ and the pion energy can be extracted from the asymptotic behavior of the two-point pseudoscalar correlation function.

### 3. Lattice computation

This work is based on a subset of the $n_f = 2$ CLS (Coordinated Lattice Simulations) ensembles generated using the nonperturbatively $\mathcal{O}(a)$-improved Wilson-Clover action for fermions and the plaquette gauge action for gluons. As shown in Table 1, three lattice spacings in the range [0.05-0.075] fm are considered with pion masses down to 193 MeV and $Lm_{\pi} > 4$ such that volume effects are expected to be negligible [17]. For more details on the ensembles, see [19]. The connected part of the three-point correlation function in Eq. (2.3) has been computing using one ‘local’ vector current $J^I_\mu(x) = \sum_f Q_f \overline{\psi}_f(x) \gamma_\mu \psi_f(x)$ and one ‘point-split’ vector current

$$J^I_\mu(x) = \frac{\sum_f Q_f}{2} (\overline{\psi}_f(x + a\vec{u})(1 + \gamma_\mu) U^I_\mu(x) \psi_f(x) - \overline{\psi}_f(x)(1 - \gamma_\mu) U^I_\mu(x) \psi_f(x + a\vec{u})), \quad (3.1)$$

whereas the disconnected part is computed using two local vector currents. In the $\mathcal{O}(a)$-improved theory, the renormalized currents read $J^a_R(\mu)(x) = Z^a_\mu(1 + b^a_\mu(x_0) a m_\mu)/(J^a_\mu(x) + a c^a_\mu T^a_\mu)$ with $\alpha = (\text{local, conserved})$ and where $b^a_\mu$ and $c^a_\mu$ are improvement coefficients. The point-split vector current satisfies the Ward identity and does not need any renormalization factor: $Z^I_\mu = 1, b^I_\mu = 0$ whereas $Z^I_\nu$ has been computed non-perturbatively in [18, 19]. We neglect the contribution from the tensor density $T^I_{\mu\nu}(x)$ such that $\mathcal{O}(a)$-improvement is only partially implemented. We choose the pion reference frame, $\vec{p} = 0$, where both photons have back-to-back spatial momenta ($\vec{q}_2 = -\vec{q}_1$) and the kinematical range accessible on the lattice can be parametrized by

$$q_1^2 = \omega_1^2 - \vec{q}_1^2, \quad q_2^2 = (m_{\pi} - \omega_1)^2 - \vec{q}_1^2.$$

We consider multiple values of $\vec{q}_1$ to obtain virtualities up to $|q_1^2| \approx 1.5 \text{ GeV}^2$ as can be seen in Fig. 1. In this kinematical setup and using the Lorentz structure of the form factor one can show that only the spatial components are non-zero and can be written

$$A_{kl}(\tau) = -i q_{kl} A(\tau), \quad q_{kl} = \epsilon_{kl\alpha\beta} q_1^\alpha q_2^\beta = m_{\pi} \epsilon_{kl} q_1^1, \quad (3.2)$$

where $A(\tau)$ is a scalar under the spatial rotation group ($\tilde{A}(\tau)$ is defined in the same way).
where the result using the lowest meson dominance model (LMD) 

\[ \tilde{A}(\tau) = 2 \left( \frac{q_1}{q_2} \right)^2 \] 

Using \( \alpha = 1/(4\pi^2 F_{\pi}) = 0.274 \text{ GeV}^{-1} \), it reproduces the anomaly constraint in the chiral limit. This model is also compatible with the Brodsky-Lepage behavior (1.1) in the single-virtual case but
folds off faster than the OPE prediction (1.2) in the double-virtual case. To reduce the number of fit parameters, a global fit is performed where all lattice ensembles are fitted simultaneously assuming a linear dependence in both $a/a_\beta=5.3$ and $\tilde{y}=m_\pi^2/8\pi^2F_\pi^2$ for each parameter of the model. We obtain at the physical point

$$\alpha^{\text{VMD}} = 0.243(18) \text{ GeV}^{-1}, \quad M_V^{\text{VMD}} = 0.944(34) \text{ GeV}. \quad (4.2)$$

As can be seen in Fig. 2, the VMD model leads to a poor description of our data ($\chi^2/\text{d.o.f.} = 2.9$, uncorrelated fit), especially in the double virtual case and at large Euclidean momenta. The second model, the LMD model [20], can be parametrized as

$$F_{\pi\gamma^*\gamma^*}^{\text{LMD}}(q_1^2, q_2^2) = \frac{\alpha M_V^4 + \beta (q_1^2 + q_2^2)}{(M_V^4 - q_1^2)(M_V^4 - q_2^2)}. \quad (4.3)$$

Again, this model reproduces the anomaly constraint and is now compatible with the OPE asymptotic behaviour where $\beta = -F_\pi/3$ is the theoretical preferred estimate (see Eq. 1.2). However, this model does not reproduce the Brodsky-Lepage behavior for the single-virtual form factor given in Eq. (1.1). Using $\alpha$, $\beta$ and $M_V$ as free parameters, we now obtain

$$\alpha^{\text{LMD}} = 0.275(18)(3) \text{ GeV}^{-1}, \quad \beta = -0.028(4)(1) \text{ GeV}, \quad M_V^{\text{LMD}} = 0.705(24)(21) \text{ GeV}, \quad (4.4)$$

with $\chi^2/\text{d.o.f.} = 1.3$ (uncorrelated fit) (Fig. 2). The first error is statistical and the second error include systematics as discussed in [14]. Although this model fails to reproduce the Brodsky-Lepage behavior, it gives a good description of our data in the considered kinematical range. The anomaly is recovered with a statistical error of 7% and $\beta$ is compatible with the OPE asymptotic result given in Eq. (1.2). Finally, the LMD+V model, proposed in Ref. [21], includes a second vector resonance and can be parametrized by

$$F_{\pi\gamma^*\gamma^*}^{\text{LMD+V}}(q_1^2, q_2^2) = \frac{\tilde{h}_0 q_1^2 q_2^2 (q_1^2 + q_2^2) + \tilde{h}_1 (q_1^2 + q_2^2)^2 + \tilde{h}_2 q_1^2 q_2^2 + \tilde{h}_3 M_V^4 M_V^4 (q_1^2 + q_2^2) + \alpha M_V^4 M_V^4}{(M_V^4 - q_1^2)(M_V^4 - q_1^2)(M_V^4 - q_2^2)(M_V^4 - q_2^2)}. \quad (4.5)$$
One main advantage of this model is that it fulfils all the theoretical constraints discussed in Sec. 1 if one sets $\tilde{h}_1 = 0$ (which is explicitly done in our fits) and $\tilde{h}_0 = -F_\pi/3$. In Ref. [21], the masses are set to their physical values $M_{V_1} = m_\rho^{\exp} = 0.775$ GeV and $M_{V_2} = m_\rho^{\exp} = 1.465$ GeV. The parameter $\tilde{h}_2 = 0.327$ GeV can be fixed by comparing with the subleading term in the OPE in Eq. (1.2) (Ref. [22, 11]) and the parameter $\tilde{h}_5 = -0.166(6)$ GeV has been determined in Ref. [21] by a fit to the CLEO data [7] for the single-virtual form factor. To get stable fits, we enforce the constraint $M_{V_1} = m_\rho^{\exp}$ at the physical point but still allowing for chiral corrections. For $M_{V_2}$, inspired by quark models, we assume a constant shift in the spectrum and set $M_{V_2}(\tilde{y}) = m_\rho^{\exp} + M_{V_1}(\tilde{y}) - m_\rho^{\exp}$. Finally, we impose the theoretical constraint $\tilde{h}_0 = -F_\pi/3$ in the continuum and chiral limit but, again, still allowing for chiral and lattice artefacts corrections. Using these assumptions, we obtain

$$\alpha^{LMD+V} = 0.273(24)(7) \text{ GeV}^{-1}, \quad \tilde{h}_2 = 0.345(167)(83) \text{ GeV}^3, \quad \tilde{h}_5 = -0.195(70)(34) \text{ GeV}, \quad (4.6)$$

with $\chi^2/\text{d.o.f.} = 1.4$ (uncorrelated fit). This model also gives a good description of our data as can be seen in Fig. 2 and turns out to be close to the LMD model in the kinematical range considered here. The systematic error has been estimated by varying our assumptions on $M_{V_1}$ and $M_{V_2}$. Again, the anomaly constraint is recovered within statistical error bars and the values of $\tilde{h}_2$ and $\tilde{h}_5$ are in good agreement with phenomenology.

The form factor extrapolated to the physical point for each model is shown in Fig. 3. In the single-virtual case, the VMD and LMD+V models are in good agreement with the experimental data whereas the LMD model starts to deviate at $Q^2 = 1$ GeV$^2$. In the double-virtual case, the LMD and LMD+V models are similar and already close to their asymptotic behavior at $Q^2 \sim 1.5$ GeV$^2$ where we have lattice data. Finally, using the formalism developed in Ref. [1] and our result for the form factor, we estimate the pion-pole contribution $a^{hLbL;\pi^0}_\mu$ to hadronic light-by-light scattering in the muon $g = 2$. Our preferred estimate for $a^{hLbL;\pi^0}_\mu$ is obtained with the fitted LMD+V model [14],

$$a^{hLbL;\pi^0}_\mu;LMD+V = (65.0 \pm 8.3) \times 10^{-11}. \quad (4.7)$$

For comparison, most model calculations yield results in the range $a^{hLbL;\pi^0}_\mu = (50 - 80) \times 10^{-11}$ with rather arbitrary, model-dependent error estimates, see Refs. [1, 12, 6] and references therein.

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