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Lattice calculation of the pion transition form factor $\pi^0 \to \gamma^* \gamma^*$

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We calculate the pion transition form factor $\mathscr{F}_{\pi^0\gamma^*\gamma^*}(q_1^2, q_2^2)$, 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 $g-2$, $a_\mu^{\mathrm{HLbL};\pi^0}$. 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 determinaiton of $a_\mu^{\mathrm{HLbL};\pi^0}$.

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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: $\gamma^*\gamma^* \to \pi^0, \eta, \eta'$ and $\gamma^*\gamma^* \to \pi^+\pi^-, \pi^0\pi^0$. 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 $a_\mu^{\mathrm{HLbL};\pi^0}$ 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

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

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

$$M_{\mu\nu} = (i^{n_0})M_{\mu\nu}^{\mathrm{E}}, \quad M_{\mu\nu}^{\mathrm{E}} \equiv -\int \mathrm{d}\tau\, e^{\omega_1\tau} \int \mathrm{d}^3z\, e^{-i\vec{q}_1\vec{z}}\, \langle 0|T\left\{J_\mu(\vec{z},\tau)J_\nu(\vec{0},0)\right\}|\pi(p)\rangle\,, \tag{2.2}$$

where ω_1 is a real free parameter such that $q_1 = (\omega_1, \vec{q}_1)$ 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

$$C^{(3)}_{\mu\nu}(\tau, t_\pi) = a^6 \sum_{\vec{x},\vec{z}} \left\langle T\left\{ J_\mu(\vec{z}, t_i) J_\nu(\vec{0}, t_f) P^\dagger(\vec{x}, t_0) \right\} \right\rangle e^{i\vec{p}\vec{x}} \, e^{-i\vec{q}_1\vec{z}} \,, \tag{2.3}$$

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_π limit. By defining

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

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

$$M^{\mathrm{E}}_{\mu\nu} = \frac{2E_\pi}{Z_\pi} \left(\int_{-\infty}^{0} \mathrm{d}\tau \, e^{\omega_1 \tau} A_{\mu\nu}(\tau) \, e^{-E_\pi \tau} + \int_{0}^{\infty} \mathrm{d}\tau \, e^{\omega_1 \tau} A_{\mu\nu}(\tau) \right) = \frac{2E_\pi}{Z_\pi} \int_{-\infty}^{\infty} \mathrm{d}\tau \, e^{\omega_1 \tau} \widetilde{A}_{\mu\nu}(\tau) \,, \tag{2.5}$$

where the overlap factor Z_π 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 $J^l_\mu(x) = \sum_f Q_f \, \overline{\psi}_f(x) \gamma_\mu \psi_f(x)$ and one 'point-split' vector current

$$J^c_\mu(x) = \sum_f \frac{Q_f}{2} \left(\overline{\psi}_f(x + a\hat{\mu})(1 + \gamma_\mu) U^\dagger_\mu(x) \psi_f(x) - \overline{\psi}_f(x)(1 - \gamma_\mu) U_\mu(x) \psi_f(x + a\hat{\mu}) \right) \,, \tag{3.1}$$

whereas the disconnected part is computed using two local vector currents. In the $\mathcal{O}(a)$-improved theory, the renormalized currents read $J^{\alpha,R}_\mu(x) = Z^\alpha_V (1 + b^\alpha_V(g_0) a m_q) \left(J^\alpha_\mu(x) + a c^\alpha_V \partial_\nu T_{\mu\nu} \right)$ with $\alpha =$ (local, conserved) and where b^α_V and c^α_V are improvement coefficients. The point-split vector current satisfies the Ward identity and does not need any renormalization factor: $Z^{c,I}_V = 1$, $b^{c,I}_V = 0$ whereas Z^l_V has been computed non-perturbatively in [18, 19]. We neglect the contribution from the tensor density $T_{\mu\nu}(x)$ 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 $|q^2_{1,2}| \approx 1.5$ 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

$$A_{kl}(\tau) = -i q_{kl} A(\tau) \,, \qquad q_{kl} \equiv \varepsilon_{kl\alpha\beta} \, q_1^\alpha \, q_2^\beta = m_\pi \, \varepsilon_{kli} \, q_1^i \,, \tag{3.2}$$

where $A(\tau)$ is a scalar under the spatial rotation group ($\widetilde{A}(\tau)$ is defined in the same way).

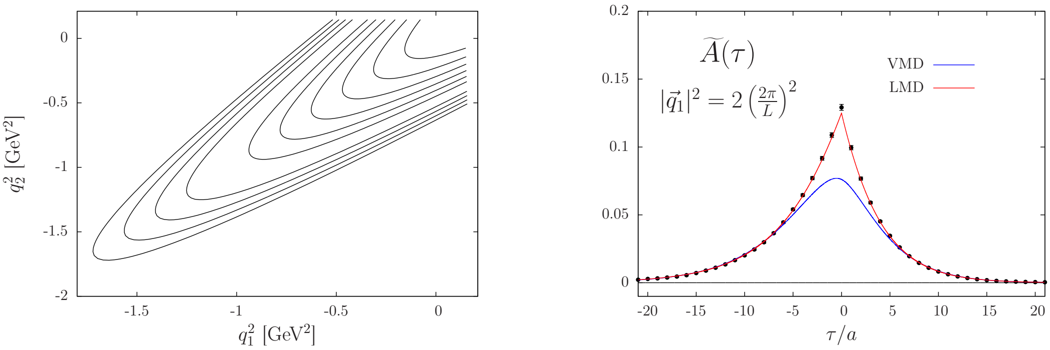

Figure 1: (left) Kinematic reach in the photon virtualities (q_1^2, q_2^2) in our setup with the pion at rest, for the lattice resolution $48^3 \times 96$ at $a = 0.065$ fm. (Right) The function $\widetilde{A}(\tau)$ (black points) and the VMD (blue line) and LMD (red line) fits used to describe the tail of the function at large τ for the lattice ensemble F7.

Table 1: Parameters of the simulations: the bare coupling $\beta = 6/g_0^2$, the lattice resolution, the hopping parameter κ, the lattice spacing a in physical units extracted from [19].

CLS	β	$L^3 \times T$	κ	a (fm)	m_π (MeV)	F_π (MeV)	$m_\pi L$	#confs
A5	5.2	$32^3 \times 64$	0.13594	0.0749(8)	334(4)	106.0(6)	4.0	400
B6		$48^3 \times 96$	0.13597		281(3)	102.3(5)	5.2	400
E5	5.3	$32^3 \times 64$	0.13625	0.0652(6)	437(4)	115.2(6)	4.7	400
F6		$48^3 \times 96$	0.13635		314(3)	105.3(6)	5.0	300
F7		$48^3 \times 96$	0.13638		270(3)	100.9(4)	4.3	350
G8		$64^3 \times 128$	0.136417		194(2)	95.8(4)	4.1	300
N6	5.5	$48^3 \times 96$	0.13667	0.0483(4)	342(3)	105.8(5)	4.0	450
O7		$64^3 \times 128$	0.13671		268(3)	101.2(4)	4.2	150

4. Results

4.1 Extraction of the form factor

In Eq. (2.5), the time integration is performed using numerical data up to $\tau_c \approx 1.3$ fm. For $\tau > \tau_c$, the contribution of the tail is estimated from a fit of our data with the analytical expression of $A_{kl}^{\mathrm{VMD}}(\tau)$ in the vector meson dominance model (VMD), derived in [14] (see the next subsection for a description of the models). A typical fit for the lattice ensemble F7 is depicted in the right panel of Fig. 1 where the result using the lowest meson dominance model (LMD) [20] rather that the VMD is also shown. Finally, the disconnected contribution to the three-point correlation function has been computed for the lattice ensemble E5 and only for the first three values of the spatial momentum $|\vec{q}_1|^2 = n^2(2\pi/L)^2$, $n^2 = 1,2,3$. It contributes to less than 1% of the total contribution and we conclude that the disconnected contribution is negligible at our level of accuracy.

4.2 Fits in four-momentum space

We first compare our results with the VMD model, parametrized by

$$\mathcal{F}_{\pi^0\gamma^*\gamma^*}^{\mathrm{VMD}}(q_1^2, q_2^2) = \frac{\alpha M_V^4}{(M_V^2 - q_1^2)(M_V^2 - q_2^2)} \,. \tag{4.1}$$

Using $\alpha = 1/(4\pi^2 F_\pi) = 0.274$ 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

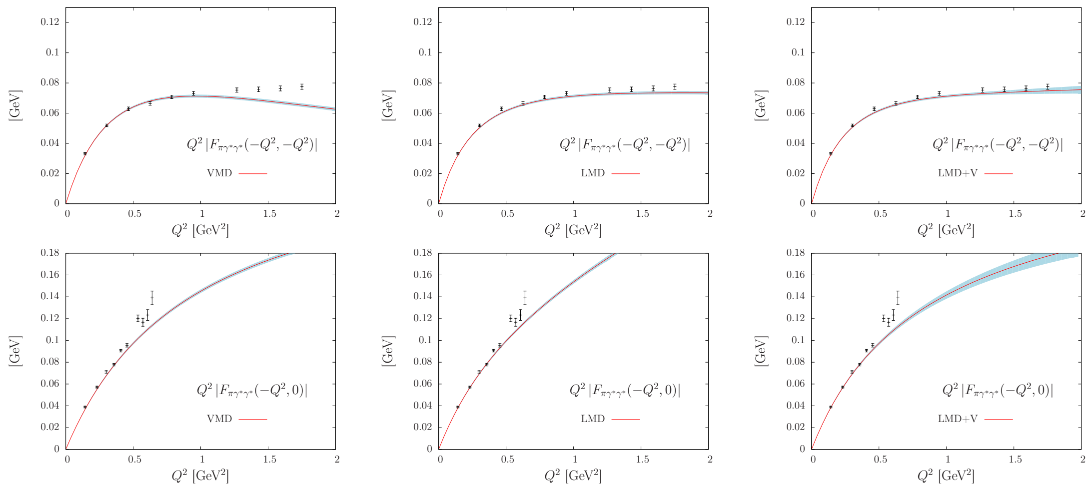

Figure 2: Comparison of the VMD, LMD and LMD+V fits for the lattice ensemble O7. The red line corresponds to the results from our global fit. The VMD model falls-off as $\mathcal{F}^{\rm VMD}_{\pi^0\gamma^*\gamma^*}(-Q^2,-Q^2) \sim 1/Q^4$ in the double virtual case and fails to describe the numerical data. Note that points at different Q^2 are correlated.

falls 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 $\widetilde{y} = m_\pi^2/8\pi^2F_\pi^2$ for each parameter of the model. We obtain at the physical point

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

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

$$\mathcal{F}^{\rm LMD}_{\pi^0\gamma^*\gamma^*}(q_1^2,q_2^2) = \frac{\alpha M_V^4 + \beta(q_1^2+q_2^2)}{(M_V^2-q_1^2)(M_V^2-q_2^2)}\,. \tag{4.3}$$

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 α, β and M_V as free parameters, we now obtain

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

with $\chi^2/\mathrm{d.o.f.} = 1.3$ (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 β 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

$$\mathcal{F}^{\rm LMD+V}_{\pi^0\gamma^*\gamma^*}(q_1^2,q_2^2) = \frac{\widetilde{h}_0\, q_1^2q_2^2(q_1^2+q_2^2) + \widetilde{h}_1(q_1^2+q_2^2)^2 + \widetilde{h}_2\, q_1^2q_2^2 + \widetilde{h}_5 M_{V_1}^2M_{V_2}^2\,(q_1^2+q_2^2) + \alpha\, M_{V_1}^4M_{V_2}^4}{(M_{V_1}^2-q_1^2)(M_{V_2}^2-q_1^2)(M_{V_1}^2-q_2^2)(M_{V_2}^2-q_2^2)}\,. \tag{4.5}$$

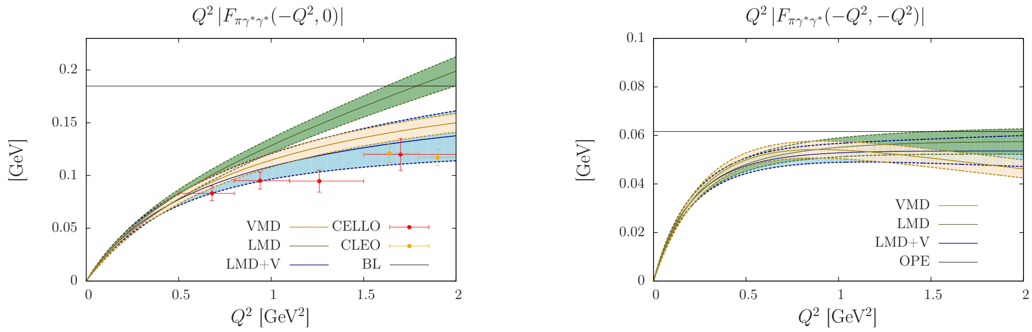

Figure 3: Lattice extrapolations for the VMD, LMD and LMD+V models. (left) Single-virtual form factor. (right) Double-virtual form factor at $Q_1^2 = Q_2^2$.

One main advantage of this model is that it fulfils all the theoretical constraints discussed in Sec. 1 if one sets $\widetilde{h}_1 = 0$ (which is explicitly done in our fits) and $\widetilde{h}_0 = -F_\pi/3$. In Ref. [21], the masses are set to their physical values $M_{V_1} = m_\rho^{\rm exp} = 0.775$ GeV and $M_{V_2} = m_{\rho'}^{\rm exp} = 1.465$ GeV. The parameter $\widetilde{h}_2 = 0.327$ GeV^3 can be fixed by comparing with the subleading term in the OPE in Eq. (1.2) (Ref. [22, 11]) and the parameter $\widetilde{h}_5 = -0.166(6)$ 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 $M_{V_1} = m_\rho^{\rm exp}$ 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 $M_{V_2}(\widetilde{y}) = m_{\rho'}^{\rm exp} + M_{V_1}(\widetilde{y}) - m_\rho^{\rm exp}$. Finally, we impose the theoretical constraint $\widetilde{h}_0 = -F_\pi/3$ in the continuum and chiral limit but, again, still allowing for chiral and lattice artefacts corrections. Using these assumptions, we obtain

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

with $\chi^2/{\rm d.o.f.} = 1.4$ (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 $\widetilde{h}_2$ and $\widetilde{h}_5$ 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 $a_\mu^{{\rm HLbL};\pi^0}$ to hadronic light-by-light scattering in the muon $g-2$. Our preferred estimate for $a_\mu^{{\rm HLbL};\pi^0}$ is obtained with the fitted LMD+V model [14],

$$a_{\mu;{\rm LMD+V}}^{{\rm HLbL};\pi^0} = (65.0 \pm 8.3) \times 10^{-11}\,. \tag{4.7}$$

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

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