Phenomenology of bivariate approximants: the $\pi^0 \rightarrow e^+e^-$ case and its impact on the electron and muon $g-2$

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The current 3σ discrepancy between experiment and Standard Model predictions for $\pi^0 \rightarrow e^+e^-$ is reconsidered using the Padé Theory for bivariate functions, the Canterbury approximants. This method, used here for the first time, provides a model-independent data-driven approximation to the decay. It implements the correct QCD constraints both at low- and high-energies to the doubly virtual $\pi^0$ transition form factor, which drives the decay. We reassess the Standard Model result including, for the first time, a systematic error. Our result, $\text{BR}(\pi^0 \rightarrow e^+e^-) = (6.20-6.41)(4) \times 10^{-8}$, still represents a discrepancy larger than 2σ, unsurmountable with our present knowledge of the Standard Model, and would claim New Physics if the experimental result is confirmed by a new measurement. Our method also provides the adequate tool to extract the doubly virtual form factor from experimental data on the double virtuality in a straightforward manner. This measurement would further shrink our window and establish once and for all the New Physics nature of the discrepancy. In addition, we remark the challenge that this rare decay poses in the evaluation of the hadronic light-by-light scattering contribution to the $(g-2)_{\mu}$, specially confronted with the foreseen accuracy of the forthcoming $(g-2)_{\mu}$ experiments.

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Pseudoscalar decays into lepton pairs provide a unique environment for testing our knowledge of QCD. As such decays are driven by a loop process, they encode, at once, low and high energies. For the $\pi^0$ decay, the process (neglecting electroweak corrections) proceeds (Fig. 1) through the $\pi^0 \rightarrow \gamma^*\gamma^*$ anomalous vertex [1], with the photons linked by a lepton line. The loop does not diverge due to the presence of the $\pi^0$ transition form factor (TFF) on the anomalous vertex, the $F_{\pi^0\gamma\gamma^*}(k^2,(q-k)^2)$ with $k^2, (q-k)^2$ space-like photon virtualities. The TFF
describe the effect of the doubly virtuality, normally represented by the product of single-virtual TFFs. The discrepancy among different approaches reflects the model-dependency of that procedure.

In this letter, we explore for the first time the role of the bivariate Padé approximants, the so-called Canterbury approximants (CA) [2], to describe in a model-independent and data-driven approach the doubly virtual TFF driving the rare decay. This technic can be generalized straightforwardly to other processes involving analytic functions with two variables.

The most accurate measurement of the $\pi^0 \rightarrow e^+e^-$ was performed by the KTeV Collaboration at Fermilab through the observation of almost 800 $\pi^0 \rightarrow e^+e^-$ events [5] and yielded $\text{BR}(\pi^0 \rightarrow e^+e^-) = (7.48 \pm 0.29 \pm 0.25) \times 10^{-8}$ after removing the final state radiative corrections (RC) [6], where the first error referred to statistics and the second to the total systematics.

The normalized $\text{BR}(\pi^0 \rightarrow e^+e^-)$ is defined as

$$
\frac{\text{BR}(\pi^0 \rightarrow e^+e^-)}{\text{BR}(\pi^0 \rightarrow \gamma\gamma)} = 2 \left( \frac{\alpha_{\text{em}} m_e}{\pi m_{\pi^0}} \right)^2 \frac{\beta_e |A(m_{\pi^0})|^2}{1 - (1 - 4 m_e^2 / m_{\pi^0}^2)^{1/2}}
$$

where $\beta_e = (1 - 4 m_e^2 / m_{\pi^0}^2)^{1/2}$ is the outgoing lepton velocity and $A(m_{\pi^0})$ is given by the loop integral

$$
A(q^2) = 2i \int \frac{dk}{\pi^2} \frac{q^2 k^2 - (qk)^2}{q^2 k^2 (q-k)^2 (p-k)^2} \tilde{F}_{\pi^0\gamma\gamma}(k^2, (q-k)^2)
$$

and encodes all the hadronic effects through the normalized TFF $\tilde{F}_{\pi^0\gamma\gamma}(k^2, (q-k)^2)$ (i.e. $\tilde{F}_{\pi^0\gamma\gamma}(0,0) = 1$). Even without any information about the TFF, Cutkosky rules may be used to extract its imaginary part, which provides the well-known unitary bound discussed by Drell [7], $\text{BR}(\pi^0 \rightarrow e^+e^-) \geq \text{BR}(\text{unitary}(\pi^0 \rightarrow e^+e^-)) = 4.09 \times 10^{-8}$, which is a model-independent result.

FIG. 1: Feynman Diagram for $\pi^0 \rightarrow e^+e^-$ process.

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The presence of the photon propagators (cf. Fig. 1) implies the kernel of the loop integral (2) to be peaked at very low energies of around the electron mass as is shown in Fig. 2. The kernel can be expanded in terms of $m_e/m_{\pi^0}$ as well as $m_e/\Lambda$ and $m_{\pi^0}/\Lambda$, being $\Lambda$ the cut-off of the loop integral, or the hadronic scale driven by the TFF. Then, Eq. (2) reads (3):

$$A(m_{\pi^0}^2) = \frac{i\pi}{2\beta_e} L + \frac{1 - \beta_e}{\beta_e} \left( \frac{1}{4} L^2 + \frac{\pi^2}{12} + Li_2 \left( \frac{\beta_e - 1}{1 + \beta_e} \right) \right) - \frac{5}{4} \int_0^\infty \frac{dQ}{Q} \left( \frac{m_{\pi^0}^2}{m_e^2 + Q^2} - \tilde{F}_{\pi^0\gamma\gamma}(Q^2, Q^2) \right)$$

where $L = \ln \left( \frac{1 - \beta_e}{1 + \beta_e} \right)$ and terms of $O \left( \frac{m_{\pi^0}^2}{m_e^2}, \frac{m_{\pi^0}^2}{m_e^2} \ln \frac{m_{\pi^0}^2}{m_e^2} \right)$ as well as $O \left( \frac{m_{\pi^0}^2}{\Lambda^2}, \frac{m_{\pi^0}^2}{\Lambda^2} \ln \frac{m_{\pi^0}^2}{\Lambda^2} \right)$ have been neglected.

The integral in Eq. (3), Fig. 2 produces a negative, diminishing the result. Omitting such contribution, Eq. (3) would result in $19 \times 10^{-8}$ for the BR.

Recently, the authors of [9] resummed the power corrections using the Mellin-Barnes technique and found the SM value at about $2\%$. Then, using a Vector Meson Dominance for the TFF, they found $BR(\pi^0 \to e^+e^-) = (6.23 \pm 0.09) \times 10^{-8}$, $3.2\sigma$ off the KTeV result.

Such discrepancy demands further explanations provided that future experiments (for example, the NA48/2 or NA62 experiments at the CERN SPS [11]) would confirm the current measurement. Three research lines can be conceived: a reevaluation of the radiative corrections, an improved parameterization of the doubly virtual TFF, or a new mechanism within physics beyond the SM [12, 13].

In Ref. [15], the radiative corrections used by the KTeV based on Bergström’s work [6] were reconsidered. At that time, Bergström considered the two-loop QED radiative correction to the decay in the soft-photon approximation, together with an inclusion of a certain cut-off for the loop diagrams. He also considered the role of the Dalitz decay and its interference as a source of experimental error. The authors of [15] noticed that [6] neglected a class of subleading diagrams, which due to particular cancellations among the dominant ones, turned out to be dominant. Later on, they also studied the role of the soft-photon approximation finding it accurate enough [15]. Ref. [6] suggests that the radiative corrections represented a $-15\%$ effect, so increasing the value measured by KTeV (see [5] for details). The reanalysis of Refs. [15] suggested, however, that including the subleading diagrams the RC would decrease down to $-6\%$, implying a smaller BR after RC are removed. With such considerations, the new KTeV value would result in $BR_{KTeV}(\pi^0 \to e^+e^-) = (6.87 \pm 0.36) \times 10^{-8}$, closer to the SM value at about $2\sigma$.

As we stated before, we investigate here the role of the TFF on such decay. Given the accuracy of Eq. (3), it is safe to conclude that the main contribution to the loop integral (2) happens at low space-like energies (Fig. 2). Therefore, a precise description of the doubly virtual TFF at low space-like energies is an essential starting-point for an accurate prediction, an observation overlooked so far. Moreover, we noticed that the factorization approximation for the TFF, i.e., $F(Q_1^2, Q_2^2) \equiv F(Q_1^2, 0) \times F(0, Q_2^2)$, can induce large effects. For our study, we consider the reconstruction of the TFF of double virtuality by a data driven approach. That method, model independent, is based on the theory of Padé approximants (PA) [17] extended to the double virtual case, the Canterbury approximants [4].

Canterbury approximants (CA) are rational approximants defined from double power series in variables $Q_1^2$ and $Q_2^2$ with the following properties [4]:

1. CA are symmetric with respect to $Q_1^2$ and $Q_2^2$.
2. CA reduce to the PA if $Q_1^2(Q_2^2) = 0$.
3. CA are unique.
4. CA satisfy the low-energy constrains by definition.
5. CA easily accommodate the high-energy QCD constraints.

Even though generalizations of CA are known [18-21], they will reduce to CA for the $\pi^0 \to e^+e^-$, representing the simplest and most efficient model-independent approach. In our case of study, the TFF, the first property follows trivially from Bose symmetry. On top, when one of the photon virtualities is zero, the resulting TFF can be safely approximated by a standard PA with great success [22, 23], satisfying the second CA property. As it is shown below, properties 3), 4) and 5) emerge naturally by construction.

CA, defined as $C_M \equiv C_M(x, y) = \frac{R_M(x, y)}{Q_M(x, y)}$ [4], extend PAs from one to two variables. The coefficients of $R_M(x, y) = \sum_{i,j} a_{i,j} x^i y^j$, and $Q_M(x, y) = \sum_{k,l} b_{k,l} x^k y^l$ are such that CA matches the Taylor expansion of the function $f(x, y)$ up to order $O(x^{\gamma} y^{N+\gamma})$, with $0 \leq \gamma \leq N + M$, i.e.,

$$f(x, y) = \sum_{k,l} b_{k,l} x^k y^l - \sum_{i,j} a_{i,j} x^i y^j = O(x^{\gamma} y^{N+M+1-\gamma})$$

with $x = Q_1^2$ and $y = Q_2^2$ guaranteeing, as anticipated, a correct low-energy description. The Canterbury group [4, 18, 19] demonstrated that for Stieltjes and meromorphic bivariate functions, the convergence of $C_M(Q_1^2, Q_2^2)$ is guaranteed, properties exploited here [20].
The first element on the CA sequence reads
\[ C_1(Q_1^2, Q_2^2) = \frac{a_{0,0}}{1 + b_{1,0}(Q_1^2 + Q_2^2)} + b_{1,1}Q_1^2 Q_2^2 , \]  \hspace{1cm} (5)

where Bose symmetry is already implemented \((b_{1,j} = b_{j,1})\) and \(b_{0,0} = 1\) without loss of generality. Eq. \(5\) reproduces the high-energy behavior when one photon virtuality is set to zero, the well known Brodsky-Lepage limit \([25]\), property 5) above. Knowing the Taylor expansion of the \(F(Q_1^2, Q_2^2)\), Eq. \(5\) would be unique: \(a_{0,0} = F(0, 0)\) is determined from the \(\Gamma(\pi^0 \rightarrow \gamma \gamma)\) through the relation \((4\pi\alpha)^2 a_{0,0} = 64\pi\Gamma(\pi^0 \rightarrow \gamma \gamma);\) \(b_{1,0}\) is the slope of the single virtual \(\pi^0\)-TFF \(b_\pi;\) and \(b_{1,1}\) is related to the doubly-virtual slope.

The second element on the CA sequence with the appropriate high-energy behavior results in
\[ C_2(Q_1^2, Q_2^2) = \frac{a_{0,0} + a_{1,0}(Q_1^2 + Q_2^2) + a_{1,1}Q_1^2 Q_2^2}{1 + b_{1,0}(Q_1^2 + Q_2^2) + b_{1,1}Q_1^2 Q_2^2 + b_{2,0}(Q_1^4 + Q_2^4) + b_{2,1}(Q_1^2 Q_2^2 + Q_2^4) + b_{2,2}Q_1^4 Q_2^4} , \]  \hspace{1cm} (6)

and demands the knowledge of four coefficients belonging to the double virtual sector \((a_{1,1}, b_{1,1}, b_{2,1} \text{ and } b_{2,2})\) as well as the curvature and third derivative of the single virtual TFF to match \(a_{1,0} \text{ and } b_{2,0}\). Obeying the convergence properties of the CA, \(C_2(Q_1^2, Q_2^2)\) approximates better the TFF than \(C_1(Q_1^2, Q_2^2)\). The difference among them can be taken as a way to estimate the systematic error on the approximation sequence \([20]\).

Experimental data for the doubly virtual \(F(Q_1^2, Q_2^2)\) is not available yet and we cannot extract all those terms from them. The OPE tells us that \(\lim_{Q^2 \rightarrow -\infty} F(Q^2, Q^2) \sim Q^{-2}\) and implies \(b_{1,1} = 0\) in Eq.\(5\) and \(b_{2,2} = 0\) in Eq.\(6\). If the OPE is fulfilled, no experimental information about the doubly virtual TFF is required up to the second element on the sequence, the \(C_2(Q_1^2, Q_2^2)\). On the other hand, if we impose the factorization approach to \(C_1(Q_1^2, Q_2^2)\), which means \(C_1(Q_1^2, Q_2^2) = P_0^1(Q_1^2) \times P_1^0(Q_2^2)\), we would find \(b_{1,1} = b_{2,0}^2.\)

For being on the conservative side, we consider the range \(0 \leq b_{1,1} \leq 2b_{2,0}^2\), where the lower limit is the OPE constrain and prevents as well the \(C_1(Q_1^2, Q_2^2)\) to have a divergency on the space-like region; and the upper one is twice the value implied by factorization. In calculating the BR we do not use \([3]\), but \([2]\), including in addition the SM Z-boson contribution. With such parameters, and taking the \(b_\pi\) value obtained in \([22]\), we determine a new SM range
\[ BR_{SM}(\pi^0 \rightarrow e^+ e^-) = (6.20 - 6.41)(4) \times 10^{-8} , \]  \hspace{1cm} (7)

where the two main numbers come from the ranging of \(b_{1,1}.\) The error \(\pm 4 \times 10^{-8}\) comes from \(\Gamma(\pi^0 \rightarrow \gamma \gamma)\) and \(b_\pi\) uncertainties together with the evaluation of the systematic error from our approximation. Such error is obtained after comparing the difference between the \(C_1(Q_1^2, Q_2^2)\) and \(C_2(Q_1^2, Q_2^2)\) \([22][23]\). To further shrink the window here provided, experimental data would then be very welcome. This final number represents still a deviation of the measured BR between \((3.3 - 2.8)\) or \((2.6 - 1.4)\) with RC in \([15][16]\), which we think is unsurmountable in a model-independent way with our present knowledge.

Therefore, to eventually improve on the situation, experimental data would be, as said, required. In Fig. \(3\) we plot the doubly virtual TFF for different virtualities. The blue band represents our range in \([3]\), while the purple (orange) band represents the TFF that would agree with KTeV result at 1\(\sigma\) with (without) taking into account the latest RC. A first glance on Fig. \(3\) reveals that, even without high precision data (30\% or even 50\% statistical error), these 3 scenarios could be easily distinguished, while improving our result \([7]\) would require higher precision, around \((10 - 20)\)\%. Such data may be fitted through CA, which being able to accommodate the high-energy
constraints from QCD as well, would allow to reconstruct the TFF from $Q^2 = 0$ to $\infty$ in the space-like region.

Tuning now $b_{1,1}$ in \cite{5} to reproduce the KTeV result, we investigate its impact on $(g - 2)_{\mu,\mu}$. There, the TFF plays a main role in the hadronic Light-by-Light (HLBL) contribution, where the $\pi^0$ exchange ($a_\pi^{\text{HLBL},\pi^0}$) represents its major piece \cite{27}. We obtain $a_\pi^{\text{HLBL},\pi^0} = 1.0 \times 10^{-14}$, which represents around 40% (or 60% with the new RC) of its quoted value \cite{27}. Given that
\[ a_\mu^\text{exp} - a_\mu^\text{th} = -105(81) \times 10^{-11} \]
we find $a_\mu^{\text{HLBL},\pi^0} = 13 \times 10^{-11}$, around 20% (50% if RC) of its standard expectations. This shift represents twice the foreseen experimental accuracy $(16 \times 10^{-11})$ in the future $(g - 2)_{\mu}$ experiments projected in Brookhaven and J-PARC \cite{28, 30} indicating that the current precision of the SM error on the $(g - 2)_{\mu}$ is underestimated if the $\pi^0 \to e^+e^-$ information is taken into account.

As anticipated in the introduction, tree level contributions from new physics may be relevant here as well. In our case, only pseudoscalar ($P$) and axial ($A$) channels are relevant, since interactions such as leptoquarks may be Fierz-rearranged \cite{31}, then, only pseudoscalar and axial channels will appear. The following Lagrangian
\[
\mathcal{L} = \frac{-g}{4m_W} \sum_f m_A c_f^A (\overline{f} A \gamma_5 f) + 2m_f c_f^P (\overline{f} i \gamma_5 f) P,
\]
where $g, m_W$ are the standard electroweak parameters, and $c_f^{A(P)}$ are dimensionless couplings to the fermion $f = \{u, d, e\}$, yields an additional term modifying Eq. (2)
\[
A(q^2) = A(q^0) + \frac{\sqrt{2} G_F F_\pi}{4 \alpha_{\mu} m_{\pi^0}^2} (\lambda^A + \lambda^P),
\]
where $G_F$ is the Fermi coupling constant, $F_\pi$ the pion decay constant, $\lambda^A = c_b^A (c_u^A - c_d^A)$ and $\lambda^P = c_b^P (c_u^P - c_d^P) / (1 - m_{\mu}^2 / m_{\pi^0}^2)$. As an illustration, the Z$^0$ boson ($\epsilon_{\mu e} = -c_A^H = 1, \epsilon_{\mu \mu}^H = 0$) shifts $A(q^2)$ by $-0.3\%$. Similarly, the “dark” Z model in \cite{11} would reduce the amplitude by $(-0.3\%) \delta^2$, with $\delta^2 \ll 1$ \cite{32}. Therefore, more general NP approaches would be required when considering axial interactions \cite{12}. Besides, pseudoscalars contributions appear in extended Higgs sectors, such as the supersymmetric model in Ref. \cite{13}. These may become large enough for $m_P \simeq m_{\pi^0}$ as may be observed from $\lambda^P$, though existing constraints discard the simplest models \cite{32}. Since many phenomenological constraints exists (dark photon searches, $(g - 2)_{e,\mu}$, electroweak physics), this represents a challenging study which is beyond the scope of this article.

In this letter, we presented a model-independent approach to describe symmetric bivariate functions based on Canterbury approximants. This method allows a model-independent study of the doubly virtual $\pi^0$-TFF in the space-like region which incorporates the low- and high-energy QCD constraints. These are essential prerequisites for calculations such as $\pi^0 \to e^+e^-$ or $a_\mu^{\text{HLBL},\pi^0}$. We found that, unless New Physics are present, the KTeV result on $\pi^0 \to e^+e^-$ implies an unexpected behavior for the doubly virtual TFF. This would produce a large shift for $a_\mu^{\text{HLBL},\pi^0}$, of the order of projected experiments for measuring $(g - 2)_{\mu}$. The effect of CAs in $\pi^0 \to 4\ell$ decays is currently under study \cite{33}. Possible effects may appear as well in $e^{+}p(\mu n)$ elastic scattering, which would be relevant for the proton radius puzzle. This situation demands an experimental measurement of $F_{\pi^0,\gamma^*,\gamma^*}$ $(Q_1^2, Q_3^2)$ as well as a new $\pi^0 \to e^+e^-$ determination.

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FIG. 3: Left panel: normalized TFF assuming $Q_1^2 = Q_2^2 = Q^2$. Right panel: normalized TFF assuming $Q_1^2 = 0.5$ GeV$^2$. Black solid line indicates the factorized TFF. Upper (blue) band shows our estimation with $0 \leq b_1 \leq 2b_1^2$. Lower (orange) band reproduces the KTeV measurement within 1σ. Middle (purple) band considers KTeV measurement with the new RC.