The electric dipole moment of the deuteron from the QCD \( \theta \)-term

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Abstract. The two-nucleon contributions to the electric dipole moment (EDM) of the deuteron, induced by the QCD \( \theta \)-term, are calculated in the framework of effective field theory up-to-and-including next-to-next-to-leading order. In particular we find for the difference of the deuteron EDM and the sum of proton and neutron EDM induced by the QCD \( \theta \)-term a value of \((-5.4 \pm 3.9) \times 10^{-17} \text{e fm}\). The by far dominant uncertainty comes from the CP- and isospin-violating \( \pi NN \) coupling constant.

PACS. 11.30.Er Charge conjugation, parity, time reversal, and other discrete symmetries – 13.40.Em Electric and magnetic moments – 24.80.+y Nuclear tests of fundamental interactions and symmetries – 21.10.Ky Electromagnetic moments

1 Introduction

Under the assumption that the CPT theorem is valid, permanent electric dipole moments (EDMs) of elementary particles and nuclei, which arise under parity \( P \) and time-reflection \( T \) breaking, belong to the most promising signals of CP-violating physics beyond the Cabibbo–Kobayashi–Maskawa (CKM) phase of the Standard Model (SM) \([1,2,9]\). Possible mechanisms \([3,4,5]\) are the dimension-four \( \theta \) vacuum angle term of Quantum Chromodynamics (QCD) \([6]\) and the effective dimension-six quark, quark-color, and gluon-color terms \([7,8,9]\) (including certain combinations of four-quark terms \([10,11]\)) resulting from extensions of the SM such as supersymmetry \([12]\), many-Higgs scenarios \([13]\) etc. In refs. \([14,15]\) it was recently pointed out that the same mechanism that drives the potential CP violation beyond the SM in \( D \to K^+ K^- / \pi^+ \pi^- \) \([16,17]\) should, if present, also lead to an enhanced nucleon EDM. However, a single successful measurement of an EDM signal of the neutron, say, would not suffice to isolate the specific CP-violating mechanism. Therefore, more than one EDM measurement involving other hadrons and (light) nuclei, \( e.g. \) the proton, deuteron, helium-3, are necessary in order to uncover the source(s) of the CP breaking.

In recent years various theoretical studies focussed on the calculation of EDMs for light nuclei \([18,19,20,21,22,23,24,25]\), largely triggered by on-going plans for dedicated experiments to measure EDMs of light ions using storage rings \([26,27,28,29,30]\). These calculations revealed that different CP-violating mechanisms contribute to different probes with different strength. Therefore, non-zero measurements as well as controlled calculations of nucleon and nuclear EDMs are necessary to reveal additional information on the physics beyond the SM that drive non-vanishing EDMs.

In this work we calculate the two-nucleon contribution to the deuteron EDM that would be produced from a non-vanishing QCD \( \theta \)-term up to next-to-next-to-leading order. Thus, once the EDMs of the proton, neutron and deuteron were measured, the results of our calculation would allow one to extract the value of \( \bar{\theta} \) directly from data, assuming that no other CP-violating mechanisms contribute significantly. Since lattice QCD will eventually be able to calculate the neutron and proton EDMs with \( \bar{\theta} \) as the only input, a combination of the calculation presented here with lattice QCD and experimental numbers will enable one to decide, if the \( \theta \)-term is the culprit of generating the EDMs. Note that direct lattice calculations for nuclear EDMs would be much more challenging.

The terms of the CP-violating interaction Lagrangian relevant for this work are given by \( \cdots \) — see ref. \([23]\) and references therein —

\[
\mathcal{L}_{\text{CP}} = \bar{N} \left( b_0 + b_1 \tau_3 \right) S^\mu N \sigma^\mu F_{\mu\nu} + g_0 \bar{N} \pi \cdot \tau N + g_1 \bar{N} \pi_3 N + C_1^0 \bar{N} N D_\mu (\bar{N} S^\mu N) + C_2^0 \bar{N} \tau N D_\mu (\bar{N} \tau S^\mu N) + C_1^1 \bar{N} \tau_3 N D_\mu (\bar{N} S^\mu N) + C_2^1 \bar{N} N D_\mu (\bar{N} \tau_3 S^\mu N) + \cdots \tag{1}
\]

Here \( v^\mu = (1,0) \), \( S^\mu = (0,1/\sigma) \) and \( \tau \) are the nucleon velocity, spin and isospin, respectively, while \( D_\mu \) is the co-
variant derivative. For $\theta$-term-induced CP violation naive dimensional analysis (NDA) gives that $g_1^\theta/g_0^\theta \sim \epsilon M_\pi^2/m_N^2$ [31]. However, as already pointed out in ref. [19] and refined further below, $g_1^\theta$ is significantly enhanced compared to this estimate — in fact, the contribution from $g_1^\theta$ dominates the deuteron EDM.

The single-nucleon EDM from the $\theta$-term starts to contribute at the one loop level [19]. At the same order there are two counter terms, proportional to $b_0$ and $b_1$, to absorb the divergence [32][33][34] — for a recent update see ref. [35]. Therefore, although the value of the CP-violating coupling constants $g_0$ and $g_1$ can be related to the strength of the QCD $\theta$-term, $\theta$, within the effective field theory the same is not possible for the EDM of a single neutron or proton. This is different in case of the nuclear EDMs: for the few-nucleon contributions, counter terms appear only at subleading orders and therefore controlled calculations become feasible, although, in case of the deuteron EDM, with a sizable uncertainty. Such subleading terms can be found in the second and third lines of eq. (1), where the two terms in third line are additionally suppressed by isospin breaking. The dots in eq. (1) denote further CP-violating terms that do not contribute to the deuteron EDM at orders considered in this work. These terms include CP-violating $NN\pi\gamma$, $NN\pi\pi\gamma$, $4N\gamma$-terms, CP-violating photon–two-pion terms, and CP-violating pure pion terms (for ref. [31] for the latter class).

There are two types of contributions that are relevant for the present study, namely CP-violating $NN$ interactions and CP-violating irreducible $NN \to NN\gamma$ transition currents — c.f. fig. 1. As will be outlined below, for the deuteron EDM the latter kind of contributions contains at its leading non–vanishing order loop diagrams that are calculated in this work for the first time.

The paper is structured as follows: in sect. 2 the prefactors of the CP-violating $\pi NN$ couplings $g_0^\theta$ and $g_1^\theta$ are derived from the QCD $\theta$-term. After this, a brief discussion of the power counting is presented in sect. 3. Section 4 contains the derivation of the two-nucleon contributions to the deuteron EDM induced by the $\theta$-term, where the $NN$ potential and transition current contributions are discussed in subsections 4.1 and 4.2 respectively. Finally, in sect. 5 a short summary of the presented results and an outlook are given. The role that the vacuum alignment plays for the generation of $g_1^\theta$ is outlined in appendix A. Appendices B and C present two further alternatives to derive the CP-violating coupling constant $g_1^\theta$, an update of the original derivation by Lebedev et al. [19] and a derivation in the framework of SU(3) chiral perturbation theory (ChPT), similarly to the one of $g_0^\theta$ by [32][33][34], respectively. Finally, appendix D is reserved for an estimate of the $g_0^\theta$ contribution resulting from a resonance-saturation mechanism involving the odd-parity nucleon-resonance $S_{11}(1535)$.

2 CP-violating $\pi NN$ couplings from the $\theta$-term

On the quark level the effect of the $\theta$-term can be written as $m_u\theta\gamma_5q$ [3], with the reduced quark mass $m_u \equiv m_u/m_d/(m_u+m_d) = (m_u+m_d)(1-\epsilon^2)/4$, where $\epsilon = (m_u-m_d)/(m_u+m_d) = -0.35 \pm 0.10$ [36]. It thus behaves under chiral rotations identically to the quark mass term and can be included in the chiral Lagrangian via

$$\chi = u^\dagger \chi u^\dagger \pm u\chi^\dagger u$$

with $\chi = 2B(s+ip)$,

(2)

where $s$ may for our purposes be identified with the quark mass matrix, which reads

$$M = \frac{m_u + m_d}{2} 1_2 + \frac{m_u - m_d}{2} \gamma_3$$

(3)

while $p = m_u \theta 1_2$. The pion fields are contained in the usual SU(2) matrix $u = \bar{U}^{1/2}$, see e.g. [37].

Starting point for the calculation of the CP-violating $\pi NN$ vertices are, to the order we are working, the quark mass dependent terms of the CP-conserving Lagrangian $\mathcal{L}_{\pi NN}^{(2)}$ [37], namely

$$c_1 N^\dagger (\chi + \bar{\chi}) N + c_5 N^\dagger \left[ \frac{1}{2} (\chi^\dagger - \overline{\chi}) \right] N$$

$$= c_1 4B(m_u+m_d) N^\dagger N$$

$$+ c_5 2B N^\dagger \left[ (m_u - m_d)\tau_3 + \frac{2m_u\theta}{F_\pi} (\pi \cdot \tau) \right] N$$

$$+ \cdots.$$ (4)

Here $\langle \cdot \rangle$ denotes the trace in flavor space. The dots indicate that terms not relevant for this study were omitted.

We start with a discussion of the term proportional to $c_5$. The first term of the third line of eq. (4) leads to
the quark-mass-induced part of the proton–neutron mass difference, \( \delta m_{\text{str}} \). It can be quantified from three different sources: (i) the use of dispersion theory to quantify the electromagnetic part of the proton–neutron mass difference \([38,39,40,41]\), (ii) lattice QCD \([42]\), or (iii) from charge-symmetry-breaking (CSB) studies of \( pn \rightarrow d\bar{\pi}^0 \) \([43]\). All analyses lead to consistent results, with the first one being the most accurate. Thus we will use \([41]\)

\[
4B(m_u - m_d)c_5 = \delta m_{\text{str}} = (2.6 \pm 0.5) \text{ MeV} .
\]  

(5)

From this we get

\[
g_0^\theta = \frac{\delta m_{\text{str}}^N(1 - \epsilon^2)}{4F_\pi \epsilon} \theta = (-0.018 \pm 0.007) \theta ,
\]

(6)

where we used \( F_\pi = 92.2 \text{ MeV} \) \([36]\). The superscript \( \theta \) indicates that we here only include the strength that comes from the \( \theta \)-term. The expression given above agrees with the prediction of ref. \([44]\) when eq. (14) of ref. \([44]\) is inserted into the corresponding eq. (8). It turns out that the value of \( g_0^\theta \) is more than a factor of 10 smaller than the estimate from NDA given by \( \bar{\theta}M_\pi^2/(m_NF_\pi) \) in terms of the pion mass \( M_\pi \), the nucleon mass \( m_N \) and the pion axial decay constant \( F_\pi \).

The first term in the second line of eq. (4) leads to the quark-mass-induced isoscalar contribution to the nucleon mass — thus \( c_1 \) can be related to the \( \pi N \) sigma term. For this low-energy constant (LEC) we use the value given in ref. \([45]\),

\[
c_1 = (-1.0 \pm 0.3) \text{ GeV}^{-1} ,
\]

(7)

which is a compilation of various extractions of \( c_1 \) \([46,47,48,49]\). At this stage this contribution does not contain a CP-odd term, however, as outlined in ref. \([50]\) and detailed within our formalism in appendix \( \mathbf{A} \) in the presence of CP violation a rotation of the vacuum is necessary in order to remove pion tadpoles from the theory. This rotation induces an additional CP-violating term in the pion–nucleon sector; namely, in agreement with ref. \([51]\) we find a coupling of \( g_1 \) type:

\[
g_1^\theta = \frac{2c_1(\delta M_\pi^2)^\text{str}(1 - \epsilon^2)}{F_\pi \epsilon} \theta ,
\]

(8)

where \( (\delta M_\pi^2)^\text{str} \) denotes the quark-mass-induced part of the mass-square-splitting between charged and neutral pions. Note that the above-mentioned vacuum rotation does produce as well a correction to \( g_0^\theta \), which, however, is numerically negligible.

Inserting the relation \([50]\)

\[
(\delta M_\pi^2)^\text{str} \approx \frac{B}{4} \frac{(m_u - m_d)^2}{m_u - (m_u + m_d)/2} \approx \frac{\epsilon^2}{4} \frac{M_\pi^4}{M_K^2 - M_\pi^2}
\]

(9)

into eq. (8) we get the result

\[
g_1^\theta \approx \frac{c_1(1 - \epsilon^2)}{2F_\pi} \frac{M_\pi^4}{M_K^2 - M_\pi^2} \theta = (0.003 \pm 0.001) \theta ,
\]

(10)

\footnote{Note that the result of ref. \([51]\) has the opposite sign to ours (which is compensated by the opposite sign of \( \epsilon \)). Furthermore, \( F_\pi \) is defined twice as large there.}

where the uncertainty of this contribution is dominated by the uncertainty in \( c_1 \). The expression given in \([10]\) exactly agrees with the one presented in appendix \( \mathbf{B} \) which is derived from \( \eta - \pi^0 \) mixing, see ref. \([19]\) and fig. 2 provided the strange-quark content of the nucleon is vanishingly small. An alternative derivation, which uses SU(3) ChPT input instead of sigma-term estimates, is presented in appendix \( \mathbf{C} \). Taking the rather large SU(3) errors into consideration, the SU(3) estimates for \( g_0^\theta \) (and \( g_1^\theta \)) are compatible with our final values which are quoted at the end of this section.

In addition to the contribution related to the \( \pi N \) sigma term there exists one additional, linearly independent operator structure that leads to a contribution to \( g_1^\theta \), see ref. \([51]\). In its notation, it is given by

\[
c_1^{(3)} = \frac{1}{4} N^\dagger (\chi_-)^2 N = c_1^{(3)} \frac{B^2 m^*(m_u - m_d)}{F_\pi} \theta N^\dagger \pi_3 N + \cdots .
\]

(11)

Unfortunately, this operator structure contributes to CP-conserving observables at too high order that it could be constrained from a study of, say, \( \pi N \) scattering. Thus we need to estimate the value of \( c_1^{(3)} \) differently. While the operator \( \chi_+ \) leads to terms that are even (odd) in the pion field for CP-conserving (violating) contributions, these relations are inverted for the operators \( \chi_- \): CP-conserving (violating) contributions are given by terms that are odd (even) in the pion field. Thus, a natural resonance saturation estimate for the operator of eq. (11) is given by a diagram, where one insertion of \( \chi_- \) converts the even-parity nucleon into the lowest odd-parity nucleon-resonance, the \( S_{11}(1535) \), which then decays via an isospin-violating decay into a neutral pion and a nucleon. The latter step may be modeled by a \( S_{11}(1535) \) decaying into \( \eta N \) which then converts into \( \pi^0 N \) via \( \eta - \pi^0 \) mixing. This contribution is potentially important, since the coupling of this nucleon resonance to \( \eta N \) is very significant \([36]\). However, an explicit calculation, see appendix \( \mathbf{D} \) shows that the mentioned contribution does not exceed the value estimated from NDA. Moreover, in order to get the proper SU(3) chiral limit of QCD, the \( \eta \) should be coupled with a derivative even to the nucleon resonances — the resulting Lagrangian is given in ref. \([51]\) — which leads to an additional suppression. We therefore consider it safe to estimate the additional \( g_1^\theta \) uncertainty due to our ignorance of \( c_1^{(3)} \) from an NDA estimate which is equal to \( \epsilon M_\pi^2/(n_N^4 F_\pi) \sim 0.002 \). In what follows we will therefore
The value of $g_1^0/g_0^0$ is numerically about a factor of 25 larger than the SU(2) estimate of order $\epsilon M^2_N/m_N$, which would follow from the first relation of eq. (12) if the scaling $\delta m_{np}^{\text{at}} \sim \epsilon M^2_N/m_N$ were assumed. The main origin of this difference is that $g_0^0$ is unusually small — instead of two powers in the counting the relative suppression numerically is of the order of one power in the expansion parameter $M_N/m_N$. It is this observation that we will use in the power counting as outlined in the next section.

### 3 Power counting

It is crucial for this study to identify a power counting that allows a comparison of the contributions to the nuclear EDMs from CP-odd transition currents to those from the CP-odd $NN$ potential. The power counting originally proposed by Weinberg for nuclear matrix elements [52] — in spite of its many successful applications, is not able to explain analogous ratios studied numerically in ref. [53] — we will therefore modify it slightly, as explained below. An alternative scheme is presented in ref. [23].

In Weinberg’s counting, contributions to the deuteron EDM that come from a CP violating potential (c.f. fig. [1]) are regarded as reducible, while the transition currents are counted as irreducible. Thus, one needs to power-count the nuclear wave functions and the photon couplings separately, making it necessary to assign a scale to a disconnected nucleon line. For dimensional reasons the corresponding $\delta^{(3)}$ function is identified with $1/p^2$, where $p$ denotes the typical momentum appearing in the evaluation of the integrals, identified with the pion mass, $M_\pi$. However, if indeed nucleon momenta are of order $M_N$, the two-nucleon intermediate state appearing between the photon coupling and the CP-violating $NN$ potential is off-shell. Thus, also this contribution is to be regarded as irreducible with the two-nucleon propagator counted as $(p^2/m_N)^{-1}$, where $m_N$ denotes the nucleon mass. Again $p$ is identified with $M_N$. This power counting properly explains the numerical observations of ref. [53] and will be used in this work as well. For more details we refer to ref. [54].

#### 3.1 Power counting for the contributions of the single-nucleon EDMs

In a world where CP violation beyond the SM is driven by the $\theta$-term, within the effective field theory the single-nucleon EDMs start at the one-loop level. At the same order there are two counter terms — the $b_i$ terms in eq. (11). The isospin structure of the loops gives that the isoscalar component of the single-nucleon EDMs is suppressed by one order in the counting compared to the isovector one [4,5]. However, this suppression is not present for the counter terms [29,33], and therefore for the power counting we may estimate both the contribution from the $d_0$ as well as the $d_1$ term from the estimate for the leading loop contribution given by

$$g_0^0 \times (M_\pi/F_\pi) \times (eM_\pi) \times (1/M_N^2) \times (M_\pi)^4/(4\pi)^2 \approx e g_0^0 F_\pi M_\pi/m_N^2 \ ,$$

where the dimension-full factors in the first line come from the regular $\pi NN$ vertex, the photon-pion vertex (with the electron charge $e < 0$), the propagators and the integration measure, respectively, and we identified $(4\pi F_\pi)^2 \sim m_N$. In order to derive from this the total transition current we need to multiply the estimate with $(1/F_\pi^2) \times m_N/M_N^2$ from the $NN$ potential and the two-nucleon propagator, respectively. We therefore find an estimate of the order of $eg_0^0/(F_\pi m_N M_\pi)$ from the single-nucleon EDM for the leading contribution to the total transition current. Thus, the single-nucleon EDMs start to contribute to the deuteron EDM at NLO, as we will outline in the next subsections — c.f. table [1].

#### 3.2 Power counting of the irreducible CP-odd $NN$ potential

The leading diagrams for the irreducible CP-odd $NN$ potential are shown in fig. [3]. The leading, isospin-conserving, CP-odd one-pion exchange can be estimated as $g_0^0/(M_N F_\pi)$. However, as will be discussed in the next section, this term does not contribute to the deuteron EDM due to selection rules. The first non-vanishing contribution comes from the subleading, isospin- and CP-odd coupling $g_1^0$. It is estimated to contribute as $g_1^0/(M_\pi F_\pi) \sim g_0^0/m_N F_\pi$, where we used the empirical relation, presented in the previous section, $g_0^0/g_0^0 \sim M_N/m_N$. This contribution will be called leading order (LO).

A CP-odd pion exchange potential from a $g_0^0$ coupling on one vertex and an isospin-odd, CP-conserving coupling on the other also leads to a non-vanishing contribution to the deuteron EDM [19,28]. As long as we focus only on contributions to the deuteron EDM, the impact of the resulting potential is effectively a redefinition $g_0^0 \rightarrow g_0^0[1 + g_0^0/2g_1^0]$, where $g_1^0$ is the strength parameter of the isospin-odd, CP-even $\pi NN$ vertex and $g_0^0$ is the axial-vector coupling constant of the nucleon. The Nijmegen partial-wave analysis provides $|\beta_1| \leq 10^{-2}$ [55], which is consistent with estimating its value from the same mechanism used in ref. [19] and appendix [8] namely via $\eta - \pi^0$ mixing — see fig. [4]. Thus the inclusion of $\beta_1$ shifts $g_0^0$ by a few percent at most and can therefore be neglected, given the significant uncertainty of $g_0^0$.

The first relativistic correction is the recoil correction to the $g_A$ vertex, given by $-g_A/(2m_N F_\pi) \cdot (p_1 + p_2) / (2k_1 \cdot a)$ where $p_{1,2}$ are the nucleon momenta and $k$ is the outgoing pion momentum. The corresponding contribution is suppressed by three orders relative to the one of the $g_A$ vertex.
In addition, also triangle topologies of type (d) as shown below, besides the latter class none of the mentioned diagrams contributes to the deuteron EDM. The CP-violating vertex is depicted by a black box. For each class of diagrams only one representative is shown.

![Diagrams](image-url)

**Fig. 3.** Contributions to the CP-violating two-nucleon potential: (a) LO contributions, (b)-(f) NLO and N^2LO contributions, where the former class contains the g_0^θ and the latter the g_1^θ coupling. Solid lines denote nucleons and dashed lines denote pions. The CP-violating vertex is depicted by a black box. For each class of diagrams only one representative is shown.

| NN potential | (total) transition current |
|--------------|---------------------------|
| LO | g_0^θ/(m_N F_π) | g_0^θ/(M_π F_π) | g_0^θ e/(M_π^2 F_π) |
| NLO | g_0^θ M_π/(m_N^2 F_π) | g_0^θ M_π/(m_N F_π) | g_0^θ e/(M_π m_N F_π) |
| N^2LO | g_0^θ M_π^2/(m_N^3 F_π) | g_0^θ M_π/(m_N^2 F_π) | g_0^θ e/(m_N^2 F_π) |

Due to the additional energy dependence (since \( v = (1, 0) \) and \( k = p_1 - p_2 \)).

To one-loop order there are a couple of diagrams as shown in fig. 3. The power counting gives for these diagrams \( g_0^θ g_0^θ/(m_N^2 F_π) \), where we identified \( 4πF_π \sim m_N \). Thus, the loop contributions with the CP-violation induced via the coupling \( g_0^θ \) by one power of \( M_π/m_N \) and therefore contribute to NLO. However, as outlined before, the spin-isospin structure of all these diagrams is such that they do not contribute to the deuteron EDM. At N^2LO the same topologies appear, however, with \( g_0^θ \) replaced by \( g_1^θ \). In addition, also triangle topologies of type (d) with the \( ππNN \) vertex from \( L_2^{(2)} \) as well as vertex corrections (diagrams (e) and (f)) formally appear at this order. As shown below, besides the latter class none of the mentioned diagrams contributes to the deuteron EDM.

On dimensional grounds CP-odd four-nucleon operators start to contribute at order \( M_π/m_N \) relative to the leading term. Their largest \( θ \)-term-induced contributions are isospin conserving (c.f. second line of eq. 1). Thus, as a consequence of the Pauli–Principle, they change the two-nucleon spin. Therefore they do not contribute to the deuteron EDM. However, their isospin-violating counter parts (c.f. third line of eq. 1) contribute, but have a relative suppression of order \( M_π/m_N^2 \) and are therefore of N^2LO.

In summary, to the order we are working, the only contribution to the CP-odd \( NN \) potential that needs to be considered for the deuteron EDM is the isospin-odd tree-level contribution proportional to \( g_0^θ \) and its vertex corrections.

### 3.3 Power counting of the irreducible transition currents

We now turn to the transition currents. As explained in the beginning of this section, in order to compare the contribution from the CP-odd \( NN \) potential to that of the CP-odd transition currents, the former needs to be multiplied by \( e/m_N/M_π^2 \). Thus, the leading order contribution of the total transition current is estimated to scale as \( g_0^θ e/m_N/(M_π^2 F_π) \sim g_0^θ e/(M_π^2 F_π) \).

The tree-level contribution, shown in fig. 4, is formally of NLO, however, turns out to be of isovector character and thus does not add to the deuteron EDM.

The one-loop contributions to the irreducible transition current are estimated as \( g_0^θ e/(m_N^2 F_π) \) and are there-
fore of $N^2\text{LO}$. The naive power counting of the diagram classes depicted in fig. 5(d) and fig. 5(e) is slightly more subtle due to the cancellation of one of the nucleon propagators by the energy dependence of the $\pi\pi\gamma$-vertex. Therefore these diagrams are part of the irreducible transition current and appear at $N^3\text{LO}$.

Finally there are two additional structures — fig. 5(k) and (l) — that appear since the zeroth component of the $\gamma\pi\pi$ vertex is proportional to the energy exchanged and thus gets sensitive to the total neutron–proton mass difference $\delta m_{np}$. The contributions of the diagrams of fig. 5(k) and (l) can be estimated as $g_0^p e \delta m_{np} / (m_N^2 F_3)$ and $g_0^p e \delta m_{np} / (m_N m_P^2 F_3)$, respectively. Thus the former (latter) appears to be suppressed by $\delta m_{np} / M_N (\delta m_{np} / m_N)$ compared to the leading order. Based on NDA one might assign $\delta m_{np} \sim \epsilon M_N^2 / m_N$ such that diagram (k) would appear at $\text{NLO}$, while diagram (l) would appear at $N^2\text{LO}$. However, as argued above the nucleon mass difference is significantly smaller than its NDA estimate — this observation made us assign $g_0^p / g_0^p \sim M_N / m_N$, and not $(M_N / m_N)^2$ as would follow from NDA. In full analogy we now assign diagram (k) and diagram (l) the orders $N^3\text{LO}$ and $N^4\text{LO}$, respectively. Therefore the former is included in our calculation while the latter can be neglected.

In Table 1 the power-counting scales of the CP-violating irreducible $NN$ potentials and those of the irreducible as well as of the total transition currents can be found. This completes the discussion of the power counting. In the next section the various diagrams are discussed explicitly.

4 EDMs from the $\theta$-term

The computation of the two-nucleon contributions to the deuteron EDM is most efficiently performed in the Breit frame defined by $q = P - P' = (0, P - P')$ where $P$ and $P'$ denote the total four-momenta of the incoming and outgoing deuteron states and $q$ the momentum of the external ‘Coulomb-like’ photon. The electric dipole moment $d$ of the deuteron nucleus of mass $m_D$ is then defined (in analogy to the magnetic moment case) by

$$d = \lim_{q \to 0} \frac{F_3(q^2)}{2m_D},$$

where the electric dipole form factor $F_3$ is related to the $P$- and $T$-violating transition current operator $(J^\text{total}_{PT})^\mu$ by

$$\langle J = 1, J_z' = \pm 1; P' | (J^\text{total}_{PT})^\mu | J = 1, J_z = \pm 1; P \rangle = \mp iq \frac{F_3(q^2)}{2m_D}.$$  

\footnote{We would like to thank J. de Vries, U. van Kolck and R. G. E. Timmermans for drawing our attention to these currents. The same effect in a different context is discussed in detail in ref. \cite{Baisou}.}
where $J$ is the total angular momentum of the deuteron and $J_i$ and $J'_i$ its $z$-components for the in- and out-state, respectively.

The total CP-violating transition current $J^\text{total}$ can be separated into two contributions of different topology (see fig. 1): two-nucleon-reducible transition currents where the P- and T-violation is induced by a CP-violating two-nucleon potential on the one hand, and irreducible CP-violating transition currents on the other. These will now be discussed in detail.

### 4.1 Contributions from the CP-odd $NN$ potential to the deuteron EDM

In order for a P- and T-violating two-nucleon potential to contribute to the deuteron channel, it must induce $^3S_1 \rightarrow ^3P_1$ transitions, i.e. isospin 0 to isospin 1 and spin 1 to spin 1 transitions since the photon-nucleon coupling is spin independent — it therefore must be antisymmetric in isospin space and symmetric in spin space.

Contributions to the CP-violating two-nucleon potential can be further separated into irreducible and reducible potentials. The latter class consists of a CP-violating potential and of multiple insertions of the $NN$ potential in the $^3S_1 \rightarrow ^3D_1$ state and/or in the intermediate $^3P_1$ state, which can be either absorbed into the deuteron wave functions, or into the intermediate $NN$ interactions in the $^3P_1$ state and therefore do not need to be considered separately.

The leading contribution to the CP-violating two-nucleon potential is the class of tree-level diagrams depicted in fig. 3(a). The tree-level potential induced by the $g_0^\theta$ vertex is given by

$$V^0_{(a)}(l) = \frac{g_0^\theta g_A}{2F_F} \frac{l}{l^2 + M^2} \cdot (\sigma(1) - \sigma(2)) \tau(1) \cdot \tau(2),$$

where $l$ denotes the pion momentum running from nucleon 1 to nucleon 2. It is spin antisymmetric and isospin symmetric and does not induce $^3S_1 \rightarrow ^3D_1$ transitions.

The potential induced by the $g_0^\theta$ vertex reads

$$V^\text{LO}_{(a)}(l) = \frac{g_0^\theta g_A}{2F_F} \frac{l}{l^2 + M^2} \left[ (\sigma(1) + \sigma(2) \tau(1) - \tau(2) \right] \right) \tau(1) \cdot \tau(2),$$

with $l$ as above. It is the same as in $10[3][10]$ with $g_0^\theta$ replaced by $g_1$. This potential-operator has a spin-symmetric and isospin-antisymmetric component and thus contributes to the transition current in the deuteron channel. In order to evaluate its contribution to the EDM of the deuteron we resort to the parametrization of the deuteron wave function of $[55]$ with a $^3D_1$-state probability of 4.8%. In order to include the $NN$ interactions in the intermediate $^3P_1$-state we use the separable rank-2 representation of the Paris nucleon-nucleon-potential of $[57]$ (PEST). The resulting contributions to the deuteron EDM listed in table 2 are in agreement with the results for $g_1$ of ref. $[20]$ using the Argonne $v_{18}$ potential, of ref. $[20][21][25]$ using the Reid93 potential, and of ref. $[18][22]$, where the deuteron wave function has been used in the Zero-Range-Approximation (ZRA). The $^3D_1$-admixture is found to enhance the deuteron EDM by about 20%, whereas the interaction in the intermediate $^3P_1$-state reduces the contribution by about the same amount.

Loops formally start to contribute at NLO. The reducible component of the box potential of fig. 3(b) constitutes a static one-pion exchange and is already accounted for either by the deuteron wave functions or by the interaction in the intermediate $^3P_1$-state. Its irreducible component may be obtained by shifting the pole of one of the nucleon propagators into the half plane of the pole of the other nucleon propagator, as outlined in $[55][59][60]$: $i/(-v \cdot p_1 + i\epsilon) \rightarrow -i/(-v \cdot p_1 + i\epsilon)$. For the sum of the irreducible part of the box potential of fig. 3(b) and the crossed-box potential of fig. 3(c), one finds in dimensional regularization in $d$ space–time dimensions

$$V^\text{LO}_{(b+c)}(l) = -i \frac{g_0^\theta g_A}{16\pi^2 F_F^3} \frac{l}{l^2 + M^2} \cdot \left[ (\sigma(1) - \sigma(2)) \tau(1) \cdot \tau(2),$$

with $\xi = l^2/(4M^2)$. Note that the divergence has been absorbed by a redefinition of the four-nucleon coupling constant $C_2^\theta$ (the scale $\mu$ is introduced in dimensional regularization).

$$C_2^0 \rightarrow C_2^0 = \frac{g_0^\theta g_A}{F_F^3} \left[ 6L - \frac{3}{16\pi^2} \left( \ln \left( \frac{\mu^2}{M^2} \right) - 1 \right) \right],$$

with

$$L = \frac{\mu^{d-4}}{16\pi^2} \left[ \frac{1}{d-4} + \frac{1}{\mu} \left[ \frac{\gamma_E - 1 - \ln(4\pi)}{2} \right]\right],$$. (20)

where $\gamma_E = 0.577215\ldots$ is the Euler–Mascheroni constant.

The triangular potential of fig. 3(d) gives

$$V^\text{LO}_{(d)}(l) = i \frac{g_0^\theta g_A}{32\pi^2 F_F^3} \sqrt{\frac{1 + \xi}{\xi}} \ln \left( \frac{\sqrt{1 + \xi} + \sqrt{\xi}}{\sqrt{1 + \xi} - \sqrt{\xi}} \right),$$

with the divergence has been absorbed by a further re-definition of $C_2^0$:

$$C_2^0 \rightarrow C_2^0 = \frac{g_0^\theta g_A}{F_F^3} \left[ -2L + \frac{3}{16\pi^2} \left( \ln \left( \frac{\mu^2}{M^2} \right) - 1 \right) \right],$$

These results reproduce those of ref. [10]. Note that all $g_0^\theta$ potential-operators up to one loop as well as the four-nucleon-vertex operators are isospin symmetric and spin antisymmetric and therefore vanish in the deuteron channel.
Table 2. Leading order contributions to the deuteron EDM from the $g_\theta^0$ vertex without $(d^0_{PW}, PW$; plane wave) and with $(d^0_{MS}$, MS; multiple scattering) intermediate $^3P_1$-interactions and the total leading order contribution $d^0_{LO}$ in units of $|g_\theta^0|/\pi F_\pi$ calculated in Zero-Range-Approximation (ZRA), with the Argonne $v_{1S}$ [61], Reid93 [22] and CD-Bonn [60] potentials.

| Potential | $d^0_{PW}$ | $d^0_{MS}$ | $d^0_{LO}$ |
|-----------|------------|------------|------------|
|           |            |            |            |
| ZRA       | $-1.8 \cdot 10^{-2}$ | $-1.8 \cdot 10^{-2}$ | |
| $A_{V_{1S}}$ | 5.76% | 5.76% | |
| Reid93    | 5.7% | 5.7% | |
| Reid93    | $-1.93 \cdot 10^{-2}$ | $0.40 \cdot 10^{-2}$ | $-1.53 \cdot 10^{-2}$ |
| This work | 4.8% | 4.8% | |

At N$^2$LO there are the same topologies as just discussed, however, with the $g_\theta^0$ vertex replaced by its isospin-violating counterpart $g_\theta^i$. The triangular-potential operator fig. 3(a) vanishes at the considered order. The class of the crossed-box-potential diagrams of fig. 3(c) gives

\[ V^{N^2LO}_{c}(t) = -i g_\theta^3 g_\theta^0 8 F_\pi^2 \left\{ \frac{1}{16 \pi^2} \frac{1 + \xi}{1 + \frac{1}{2} \xi} \ln \left( \frac{\sqrt{1 + \xi} + \sqrt{\xi}}{\sqrt{1 + \xi} - \sqrt{\xi}} \right) + 3L - \frac{3}{2} \frac{1}{16 \pi^2} \left( \ln \left( \frac{\mu^2}{M_F^2} \right) - 1 \right) - \frac{1}{16 \pi^2} \right\} \times \left\{ \left( \tau^3_{(1)} - \tau^3_{(2)} \right) (\sigma_{(1)} + \sigma_{(2)}) + \left( \tau^3_{(1)} + \tau^3_{(2)} \right) (\sigma_{(1)} - \sigma_{(2)}) \right\} \cdot \tau \cdot \mu. \tag{23} \]

Resorting again to the method presented in [58, 59, 60] to isolate the irreducible component of the box-potential operator fig. 3(b), the latter is found to be the negative of eq. (23) and to cancel the crossed-box-potential operator fig. 3(c). Therefore, contributions to the total CP-violating transition current induced by the CP-violating two-nucleon-one-loop potential are absent to N$^2$LO — not only in the deuteron channel.

The only non-vanishing N$^3$LO contributions are thus the vertex corrections shown in diagrams 3(e) and (f). The vertex correction on the CP-conserving vertex is readily accounted for, since we use the physical $\pi NN$ coupling constant in our calculations. The situation is somewhat different for diagram 3(c), where the physical value of the coupling constant is not known, but was calculated/estimated in sect. 2. Since $g_\theta^0$ only appears at the one-loop level in the case of the deuteron EDM, we only need to consider $g_\theta^0$. The quoted uncertainty for $g_\theta^0$ is of the order of 50%. On the other hand, the corresponding correction for the CP-conserving $\pi NN$ coupling constant, the so-called Goldberger-Treiman discrepancy, is very small [60], such that we may safely assume that the uncertainty given for $g_\theta^0$ is sufficiently large that it includes vertex corrections.

Thus, the only piece of the $NN$ potential that is CP odd and contributes to the deuteron EDM is the tree-level diagram depicted in fig. 3(a), with the $g_\theta^0$ coupling employed in the CP-odd $\pi NN$ vertex: it is the LO potential.

4.2 Contributions from the CP-odd irreducible $NN$ transition current

In order for an irreducible transition current not to vanish in the deuteron channel, it has to induce $^3S_1 \rightarrow ^3S_1$, $^3S_1 \rightarrow ^3D_1$ (isospin 0 to isospin 0 and spin 1 to spin 1) transitions. It therefore needs to be an isoscalar operator, symmetric in spin space. Therefore the tree-level transition currents — c.f. fig. 3(a) — that are all isovector in character, do not contribute to the deuteron EDM. The relevant CP-odd irreducible one-loop $NN$ current operators are listed in fig. 3(b). Diagrams involving CP-even $NN\gamma$-vertices have been neglected here since, to the order we are working, they do not yield EDM contributions: according to eq. (15) EDM contributions are extracted from the 0th-component of matrix elements of transition currents. The leading order, CP-even $NN\gamma$ vertex $ie(g_A/F_\pi) e \cdot S \epsilon^{a3b} \gamma^5 \gamma^\mu$ (see appendix A of [37]) does not have a non-vanishing 0th-component for $S = (0, \sigma/2)$.

The diagram classes depicted in fig. 3(g) and fig. 3(h) are of order $g_\theta^0 e/(m_N F_\pi)$ and thus N$^2$LO. For a photon coupling to nucleon 2 the two-nucleon-irreducible component of diagram fig. 3(g) and diagram fig. 3(h) give

\[ \left( \frac{g^{N^2LO}_{N+\phi}}{g^{N^2LO}_{N+\phi}} \right)^\mu = i g_\theta^3 g_\theta^0 120 \pi F_\pi^2 M_F \left[ \frac{1}{1 + \xi} + \frac{2}{\sqrt{\xi}} \arctan \sqrt{\xi} \right] e^\mu \times \left( \tau^3_{(1)} \cdot \tau^3_{(2)} - \tau^3_{(2)} \cdot \tau^3_{(1)} \right) (\sigma_{(1)} - \sigma_{(2)}) \cdot (p_2 - p_1 + q) \tag{24} \]

with $\xi = |p_2 - p_1 + q|^2 / (4M_F^2)$ in terms of the initial (final) momentum $p_i (p'_i)$ of nucleon $i$ and the momentum of the outgoing photon $q$. Although the operator (24) contains an isospin-symmetric component, it is spin-antisymmetric and vanishes in the deuteron channel.

The diagram classes depicted in fig. 3(d) and (e) vanish in the deuteron channel, since they are isovectors.

In addition there are diagrams at N$^2$LO where the photon couples to a vertex correction (fig. 3(i) and (j)); however, terms that contain the $g_\theta^0$ vertex turn out to be isovectors and thus do not contribute to the deuteron channel, and those that contain $g_\theta^i$ start to contribute only at N$^3$LO.

The triangular diagrams depicted in fig. 3(b), fig. 3(c) and fig. 3(f) are all of order N$^3$LO. Diagrams of the types of fig. 3(e) and fig. 3(f) vanish in the deuteron channel which can readily be seen from isospin components:
diagram fig. 5(c) is proportional to $\tau_2^0$ (photon coupling to nucleon 2) and diagram fig. 5(f) is proportional to $2\tau_2 + i(\tau_1 \times \tau_2)$. A class of currents that has a spin-and isospin-symmetric component is depicted in fig. 5(h):

\[
\left( g_{\text{N}^2\text{LO}} \right)_{(b)} = i \frac{g_0 g_A}{4 F^2} \tau^\mu \left( \tau_1 \cdot \tau_2 - \frac{3}{2} \tau_2 \right) \times \left( p_1 p_0^2 - p_1^2 p_0 - \sigma_{(2)} + 1 \leftrightarrow 2 \right) \quad (25)
\]

with $I(l) = -\arctan(|l| / (2M_\pi)) / (8\pi |l|)$ [37]. Resorting to the CD-Bonn wave function of the deuteron as used above, the resulting $g_0^\text{NLO}$ contribution to the deuteron EDM for the $^3S_1$ state and $^3D_1$ admixture is found to be

\[
g_{\text{N}^2\text{LO}}(b) = -2.00 \cdot 10^{-4} \times G_0^1 e\text{ fm} - 0.53 \cdot 10^{-4} \times G_0^3 e\text{ fm} \quad \text{$^3D_1$-adm.}
\]

where $G_0^1 := g_0^0 g_{\text{APN}} / F_\pi$.

The class of diagrams depicted in fig. 5(k), see ref. [28], gives

\[
\left( g_{\text{N}^2\text{LO}} \right)_{(k)} = -i \frac{g_0 g_A \lambda_{\text{np}}}{F_\pi} \tau^\mu \left( \tau_1 \cdot \tau_2 - \frac{3}{2} \tau_2 \right) \times \left[ \frac{\sigma_{(1)} \cdot (p_1 - p_1') + \sigma_{(2)} \cdot (p_2 - p_2')}{[(p_1 - p_1')^2 + M_\pi^2][(p_2 - p_2')^2 + M_\pi^2]} \right].
\]

The explicit evaluation of the EDM contribution of fig. 5(k) yields $0.31 \cdot 10^{-4} \times G_0^1 e\text{ fm}$, which justifies the classification as $N^2\text{LO}$.

The absence of both — divergences and (undetermined) counter-terms up to $N^2\text{LO}$ — ensures the predictive power of the two-nucleon contributions to the deuteron EDM that is induced by the $\theta$-term. Together with the $g_0^1$ contribution the total two-nucleon contribution to the EDM of the deuteron induced by the $\theta$-term is then given by:

\[
d^\theta = d_{\text{LO}}^\theta + d_{\text{N}^2\text{LO}}^\theta
\]

\[
= \left( -15.2 \cdot \frac{g_0^1}{g_0^0} - 0.22 \right) \pm 0.03 \times 10^{-3} G_0^1 e\text{ fm},
\]

where the uncertainty estimates the higher order contributions not included as given by the power counting. Alternatively we may express the result directly in terms of $\bar{\theta}$, the strength of the QCD $\theta$-term, and write

\[
d^\theta = d_{\text{LO}}^\theta + d_{\text{N}^2\text{LO}}^\theta
\]

\[
= -((5.9 \pm 3.9) - (0.5 \pm 0.2)) \times 10^{-4} \bar{\theta} e\text{ fm},
\]

where the uncertainties now contain, in addition to the one given in eq. [28], also the uncertainties in the coupling constants $g_0^0$ and $g_0^1$. Therefore the final result is completely dominated by the contribution from the CP- and isospin-violating tree-level potential proportional to $g_1^0$.

5 Summary and conclusions

As already stated in the introduction, the established relation between the QCD $\theta$-term and the CP-odd $\pi\eta N$ coupling constant is not sufficient to predict the size of the electric dipole moment of a single nucleon (neutron or proton) with the help of effective field theory, since the calculable one-loop contributions are of the same order as undetermined counter terms. However, this unpleasant feature is not present for the two-nucleon contributions of the deuteron and other light nuclei, which contribute already at tree-level order — unaffected by any counter terms — and which can be derived — admittedly with a large uncertainty — up-to-and-including the order $N^2\text{LO}$, see eqs. (28) and (29) at the end of sect. 4.2. The $N^2\text{LO}$ contributions of these results are (up to vertex corrections discussed in sect. 5) solely governed by the irreducible transition currents. The latter include loops which for the first time have been calculated in the present work. Note that any contribution with unknown coefficients can only show up at $N^3\text{LO}$.

The dominant part of the deuteron’s two-nucleon EDM from the QCD $\theta$-term resulted from an isospin-violating, CP-odd $\pi NN$ coupling constant, $g_1$. The isospin-violation of this coupling can be estimated from the strong contribution to the pion mass-square splitting $(\delta M_{\pi}^2)^{\text{str}} / M_\pi^2$.

This number may presumably be taken as a scale for the one-pion exchange with one $g_0^0$ vertex cannot contribute to the two-nucleon part of the deuteron EDM because of isospin selection. This was summarized in the folklore that the deuteron would be blind to the two-nucleon contributions generated by the $\theta$-term. This folklore, however, should be abandoned. A measurement of a non-vanishing neutron, a non-vanishing proton and a non-vanishing deuteron EDM would suffice to determine the strength of the QCD $\theta$-term, $\bar{\theta}$, from data. Note that the two-nucleon part of the deuteron EDM given in [29] is in fact of the same magnitude and therefore comparable in size with the non-analytic isovector part of the nucleon EDM as calculated in ref. [33], which is, using as input the value of $g_0^0$ from eq. (9),

\[
d_N^{\text{non-analyt.}} = (21 \pm 9) \times 10^{-4} \bar{\theta} e\text{ fm},
\]

where the uncertainty contains both the variation of the loop scale as proposed in ref. [33] as well as the uncertainty in $g_0^0$. This number may presumably be taken as a scale which governs the single nucleon EDMs. Note, however, that the non-analytic contribution to the isoscalar part of the nucleon EDM is an order of magnitude smaller due to a suppression by a factor $M_N / m_N$ as well as the absence of a chiral logarithm. Whether the proton or neutron EDM are really of the same magnitude as the two-nucleon part of the deuteron EDM is a question which only experiments might eventually be able to answer.
Fact is that, under the assumption that the electric dipole moments are driven by the CP violation that is induced by the QCD $\theta$-term, we now can give a relation between the total EDMs of the deuteron, the neutron and the proton and the calculated two-nucleon EDM part of the deuteron:

$$d_D = d_n + d_p - ((5.9 \pm 3.9) - (0.5 \pm 0.2)) \times 10^{-4} \, \theta \, \text{e fm.} \quad (31)$$

A cross-check of the so-extracted $\theta$ value would be possible — still solely from data — by a measurement of the EDMs of $^3$He. Another strategy to test or falsify the $\theta$ value would involve lattice QCD calculations and just two successful EDM measurements, namely one single-nucleon EDM, i.e. the one of the neutron or proton, and the deuteron EDM. If even all three of them are measured, then one could use lattice QCD for a first test correlating the proton and neutron EDM results in terms of the parameter $\theta$ and to use formula (31) for an additional, orthogonal test.

If indeed the QCD $\theta$-term would have failed these tests — either by a direct comparison of data or by the additional involvement of lattice QCD — then the following picture would emerge: in case $d_p = d_n = d_p$ is sizable compared to what eq. (31) in combination with experimental or lattice data predicts, then the dimension analysis reveals a dominance of the quark-color EDM, feeding the Lagrangian which explicitly breaks the SU(2) $\times$ SU(2) symmetry imposes a constraint on the selection of the ground state. The SU(2) subgroup to which SU(2) $\times$ SU(2) is broken is uniquely specified. This implies especially the absence of pion tadpoles. Therefore, the incorporation of CP-violating and chiral-symmetry-breaking terms into the Lagrangian requires, in general, an adjustment of the vacuum, i.e. an axial transformation $A = R = L^1$,

$$U \leftrightarrow AU \quad N \to K(A^1, A, U)N \quad (A.1)$$

with $U = u^2$ (see e.g. [67]). In the representation which we are using, the $\theta$-term is related to the isospin-breaking mass term by an axial rotation that contains $\tau_3$ only, $A = \exp(i\alpha\tau_3/2) - c.f.$ the discussion at the beginning of sect. 2. Since CP violation is a small perturbation, it will slightly shift the ground state $U_0 = 1_2$ according to $U_0 \to AU_0A$. The rotation angle $\alpha$ is determined by minimizing the potential $V$ in the vicinity of the ground state $U_0$:

$$\partial V[U = AU_0A]/\partial \alpha = 0. \quad (A.2)$$

The term $F_2^2(\chi_+)/4$ belonging to the second-order Lagrangian in the pion sector (see $L_1$ in ref. [67] would, by itself, not induce a vacuum shift (i.e. $\alpha(\theta) = 0$), since the pseudoscalar source $p$ in eq. (2) is purely isoscalar. Thus leading order tadpoles are avoided. However, the $l_2$ term of the subleading fourth-order Lagrangian in the pion sector, see $L_2$ and eq. (5.5) in ref. [67], does give rise to a $(\pi_3)$ tadpole term:

$$-\frac{l_2}{16}(\chi_-)^2 = -l_2(1 - \epsilon^2)\epsilon M_4^2 \bar{\theta} \frac{\pi_3}{F_{\pi}^2} \left(1 - \frac{2\pi_3^2}{3F_{\pi}^2}\right) + \cdots.$$  

(3.3)

Therefore, this tadpole contribution has to be canceled by a perturbative shift of the leading-order term $F_2^2(\chi_+)/4$ that is induced by an axial rotation of the ground state by the small angle

$$\alpha'(\theta) = -l_2(1 - \epsilon^2) \frac{M_4^2}{F_{\pi}^2} \bar{\theta} + \mathcal{O}(\bar{\theta}^2). \quad (A.4)$$

Note that the $L_2$ terms proportional to $l_1, l_2, l_5, l_6$ as well as to the so-called high-energy constants, see ref. [67], are invariant under the rotation $A$. Furthermore, the $L_2$ term proportional to $l_4$ does not contribute either, since here the sole external current is the electromagnetic field and since $[\chi, Q] = 0$ ($Q$: quark charge matrix). Thus there remain only higher-order contributions which are generated by the $l_3$ and $l_7$ terms of $L_2$. These contributions scale as the sixth-order order terms of the pion-sector Lagrangian, i.e. as $L_3$ in the notation of ref. [67], and can be neglected here.

Note, however, that the redefinition of the ground state also induces new structures into the pion-nucleon Lagrangian [31], namely

$$c_1(\chi_+)^N \to -4\alpha'(\theta)c_1 M_4^2 \frac{\pi_3}{F_{\pi}} \left(1 - \frac{\pi_3^2}{6F_{\pi}^2}\right) N^1N + \cdots,$$

$$c_3(\chi_+)^N \to -2\alpha'(\theta)c_3 M_4^2 \frac{\pi \cdot \tau}{F_{\pi}} \left(1 - \frac{(1 - \epsilon^2)\theta}{2\epsilon}\right) \frac{(1 - \epsilon^2)\theta}{2\epsilon} \tau_3 \theta.$$  

(3.5)

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A Selection of the ground state

As pointed out in [66] the presence of a term in the Lagrangian which explicitly breaks the SU(2) $\times$ SU(2) symmetry imposes a constraint on the selection of the ground

3 Note that ref. [23] stated the dominance of the quark-color mechanism already under the assumption that $d_D = d_n = d_p$, itself is sizable. The difference emerges since in ref. [23] the relative suppression between $g_l^p$ and $g_l^n$ was taken from naive dimensional analysis that predicts a negligible contribution from the $g_l^p$ term.
The terms proportional to $c_2, c_3, c_4, c_6$ and $c_7$ in the pion-nucleon Lagrangian are invariant under the axial rotation $A$ when the electromagnetic field is the sole external current. The $c_5,c_7$ term is proportional to $\mathcal{O}(\delta^2)$ and can be disregarded. While the remaining $c_5$ term in (A.5) provides a correction to the value of $g_0^\pi$ the term proportional to $c_5$ is a new structure: a $\delta M^2$-vertex which is driven by the low energy constant $\delta$. The latter is related to the strong-interaction part of the pion mass-square shift ($\delta M^2_{\pi}^{\text{str}}$) by [67]:

$$
\delta M^2_{\pi}^{\text{str}} := (M^2_{\pi} - M^2_{\pi}^{\text{str}}) \bigg|_{\text{strong}} = \frac{2(m_u - m_d)^2 B^2\gamma_f / F^2_\pi + \cdots}{(7 \text{ MeV})^2} \approx 2 M_\pi \cdot 0.18 \text{MeV}. \quad (A.6)
$$

This leads to eq. (A.7), i.e.

$$g_0^\pi = \frac{2 c_1}{F_\pi} (\delta M^2_{\pi}^{\text{str}} (1 - c^2)) \frac{\bar{\theta}}{\epsilon}, \quad (A.7)
$$

which agrees with the corresponding term in eq. (113) of [31]. Finally, the correction to $g_0^\pi$ is given by

$$
\delta g_0^\pi = \frac{\delta m_{\pi}^{\text{str}} (1 - c^2)}{4 F_\pi \epsilon} \frac{\bar{\theta}}{\epsilon} (\delta M^2_{\pi}^{\text{str}}) = g_0^\pi \frac{\delta M^2_{\pi}^{\text{str}}}{M^2_{\pi}}, \quad (A.8)
$$

reproducing the corresponding term in eq. (113) of [31].

B An update of the derivation of Lebedev et al. [19]

In addition to the usual parametrization of the $\theta$-term induced isospin-conserving and CP-violating $\pi NN$ coupling

$$
g_0 = \frac{m_u - m_d}{F_\pi} \langle N|\bar{u}u - \bar{d}d|N\rangle \quad (B.1)
$$

the authors of ref. [19] introduced — via the $\pi^0-\eta$ mixing — the isospin-breaking counterpart

$$
g_1^\pi = \frac{m_u - m_d}{4m_s - m_N} \frac{\bar{\theta}}{\sqrt{3}} \langle N|\bar{u}u - \bar{d}d - 2\bar{s}s|N\rangle. \quad (B.2)
$$

This is an alternative derivation of the vacuum-alignment result [A.7] for $g_1^\pi$, discussed in appendix A because the $l_7$ coefficient of the fourth-order Lagrangian effectively summarizes the $\pi^0-\eta$ mixing by the quark-mass dependent shift to the pion-mass-square ($\delta M^2_{\pi}^{\text{str}}$).

Inserting the strong-interaction contribution to the neutron-proton mass difference $(m_u - m_d) \langle N|\bar{u}u - \bar{d}d|N\rangle = \delta m_{\pi u}^{\text{str}}$ and utilizing the parameter $\epsilon$ as defined at the beginning of sect. [2] we derive [62] again:

$$
g_0^\pi \approx \frac{\delta m_{\pi u}^{\text{str}} (1 - c^2)}{4 F_\pi \epsilon} \bar{\theta}. \quad (B.3)
$$

Similarly, starting now from eq. (B.2), we get

$$
g_1^\pi = -\frac{\bar{\theta}}{8 F_\pi} (1 - c^2) \epsilon \frac{M^2_\pi}{M^2_K - M^2_\pi} \bar{\eta} \langle N|\bar{u}u + \bar{d}d - 2\bar{s}s|N\rangle \quad (B.3)
$$

with $M^2_\pi = 2 B \bar{\eta} + O(M^2)$ and $M^2_K = B(m_u + \bar{m}) + O(M^2)$ for the square of the pion and kaon mass, respectively, where here $M$ is the quark mass matrix for three light flavors. According to refs. [40,69] we have $\bar{m}_N = 0.0021 \text{MeV}$, and the $\bar{M}$ quark masses at 2 GeV from [66], we get

$$
g_0^\eta \approx (-0.018 \pm 0.007) \bar{\theta} \quad (B.5)
$$

and

$$
g_1^\eta \approx (0.0012 \pm 0.0004) \bar{\theta} \quad (B.6)
$$

with $\sigma_{\eta NN}(0) = 45 \text{MeV}$ and $y = 0.21 \pm 0.20$ from [69] as additional input. Thus we find

$$
\frac{g_1^\eta}{g_0^\eta} \approx (0.0021 \pm 0.0004) \bar{\theta} \quad \text{and} \quad \frac{g_1^\pi}{g_0^\pi} \approx -0.11 \pm 0.05 \quad (B.7)
$$

as values for $g_1^\pi$ and the ratio instead. Note that the ratios listed in (B.7) and (B.8) are compatible with the estimate [63].

C Derivation via SU(3) chiral perturbation theory

In SU(3) ChPT the $D$-type and $F$-type CP-violating $\pi^0 NN$ coupling constants are (see e.g. the U(3) ChPT calculation of ref. [31])

$$
g_{\pi^0 NN}^D = \frac{4 B \bar{\eta} m_s}{F_\pi} b_D \quad \text{and} \quad g_{\pi^0 NN}^F = \frac{4 B \bar{\eta} m_s}{F_\pi} b_F, \quad (B.9)
$$

respectively, whereas

$$
g_{\eta NN}^D = \frac{-4 B \bar{\eta} m_s}{F_\pi} \sqrt{3} b_D \quad \text{and} \quad g_{\eta NN}^F = \frac{4 B \bar{\eta} m_s}{F_\pi} \sqrt{3} b_F. \quad (B.10)
$$

---

4 Actually, via the $\pi^0-\eta$ mixing. For consistency, we replaced here their $\pi^0-\eta$ mixing angle by the customary one of chiral perturbation theory [50] — note the explicit $\bar{m}$ subtraction in the denominator.
Table 3. The value of $g_0^a$, $g_1^a$, and the ratio $g_1^a/g_0^a$ predicted from eqs. (C.1) and (C.2) with (i) the original SU(3) parameters $b_D$ and $b_F$ of ref. [37], with (ii) the alternative set of parameters based on eqs. (C.5) and (C.6), (iii) in the case that $b_D + b_F$ of (i) are replaced by $c_5$ of eq. (13). The listed uncertainties do not contain systematical SU(3) errors.

| $g_0^a / \theta$ | $g_1^a / \theta$ | $g_1^a / g_0^a$ |
|------------------|------------------|------------------|
| $b_D \& b_F$ from [37] | $-0.092 \pm 0.002$ | $-0.092 \pm 0.0017$ | $-0.036 \pm 0.007$ |
| $b_D \& b_F$ alternative | $-0.023 \pm 0.005$ | $0.00088 \pm 0.00016$ | $0.038 \pm 0.011$ |
| $b_D + b_F \rightarrow c_5$ | $-0.018 \pm 0.007$ | $0.00092 \pm 0.00017$ | $-0.051 \pm 0.022$ |

are the corresponding $\eta N N$ (actually $\eta_b N N$) counter parts. Note that $4B b_D$ and $4B b_F$ are the coefficients of the anticommutator ($D$-type) and commutator ($F$-type) term of the quark mass matrix with the baryon matrix. Therefore, the SU(3) counter parts of eqs. (9) and (13) are

$$g_0^a = \frac{4B \theta m_{bb}(b_D + b_F)}{F_5} = \epsilon_m \frac{M_3}{F_5}(1 - c^2)(b_D + b_F), \quad (C.1)$$

$$g_1^a = \frac{4B \theta m_{bb}(3b_D - b_F)}{F_5} = \frac{\epsilon_m}{\sqrt{3}} \frac{M_3}{m_s - m_{\eta}} M_3 = \frac{\epsilon_m}{\sqrt{3}} \frac{M_3}{m_s - m_{\eta}} M_3 \frac{M_3}{F_5}(1 - c^2)(3b_D - b_F), \quad (C.2)$$

where $(\sqrt{3}/4)(m_d - m_u)/(m_s - m_{\eta})$ is the $\pi^0$-$\eta_b$ mixing angle. Thus, in this case we get the ratio

$$\frac{g_1^a}{g_0^a} = \frac{\epsilon_m}{4(M_3^2 - M_3^2)} \frac{3b_D - b_F}{b_D + b_F}. \quad (C.3)$$

If the values $b_F = -0.209$ GeV$^{-1}$ and $b_D = 0.066$ GeV$^{-1}$ of ref. [37] are inserted, we get the first row of table 3. Note, however, that there is a mismatch by a factor 1.5 approximately between the SU(3) octet quantity

$$b_D + b_F = -\frac{m_\Sigma - m_\Sigma}{4(M_3^2 - M_3^2)} \approx (-0.143 \pm 0.004) \text{ GeV}^{-1}$$

used in [32,33] and the SU(2) low-energy coefficient (LEC)

$$c_5 = \frac{\delta m_{npp}}{4M_3^2} \approx (-0.097 \pm 0.034) \text{ GeV}^{-1}, \quad (C.4)$$

although according to SU(3) ChPT both quantities should agree to leading order, see eq. (27) of ref. [37].

Moreover, an alternative procedure to parametrize the above sum is

$$b_D + b_F = \frac{\delta m_{npp}}{4(M_3^2 - (M_3^2 - M_3^2) - M_3^2)} \approx (-0.126 \pm 0.024) \text{ GeV}^{-1}, \quad (C.5)$$

where the electromagnetic mass shifts are removed (via the Dashen theorem [75] in the denominator) and where the prediction falls in-between the original one and the $c_5$ value. Using an analogous parametrization for $b_F$, we get

$$b_F = \frac{m_\Sigma - m_\Sigma}{8(M_3^2 - (M_3^2 - M_3^2) - M_3^2)} \approx -0.196 \text{ GeV}^{-1} \quad (C.6)$$

and $b_D = +0.069 \pm 0.024$ GeV$^{-1}$ from (C.5) instead of the above listed values from [37], such that the values in the second row of table 3 are generated instead. Note that the result for $3b_D - b_F$ is approximately the same in both parametrizations, namely $-0.69$ GeV$^{-1}$ in the original one at and $-0.66$ GeV$^{-1}$ in the modified one.

Finally, replacing $b_D + b_F$ of [37] by $c_5$ of eq. (C.4), we get the values in the third row of table 3.

Note that only the last SU(3) value of the ratio $g_1^a/g_0^a$ is in the range of our estimate (13), but all three are compatible with the estimate of [32,33]. The quoted numbers of table 3, however, do not contain a systematical error connected with an SU(3) ChPT calculation. For standard quantities such an uncertainty is certainly of the order of 50%. For the quantity $c_5$ this uncertainty should be rather 100%--200%, see e.g. footnote 6. Taking these SU(3) errors into account, the estimates of the table 3 are compatible with the range quoted in [13].

D The contribution of the odd-parity nucleon resonance to $g_1^a$

According to ref. [38] the mass, width and $\Gamma_N$ branching ratio of the $S_{11}(1535)$ odd-parity nucleon-resonance are $m_{N_{1535}} = (1535 \pm 10) \text{ MeV}$, $\Gamma_{N_{1535}} = (150 \pm 25) \text{ MeV}$ and $B_{N_{1535} \rightarrow \eta} = (42 \pm 10) \%$. Finally the CM-momentum is $p^* = 186 \text{ MeV}$. The partial decay width $\Gamma_{N_{1535} \rightarrow \eta}$ is then approximately 63 MeV, such that one finds for the effective coupling constant for the decay $N^* \rightarrow \eta$

$$|g^a| = \sqrt{\frac{8\pi \Gamma_{N_{1535} \rightarrow \eta}}{p^*}} \approx 2.9, \quad (D.1)$$

where we assumed an energy-independent decay vertex. By inserting

$$\frac{1}{\sqrt{2}} (i \chi_{-}) = -\frac{M_3}{2} (1 - \epsilon^2) \theta (1 - \frac{\eta}{F_5}) + \epsilon \frac{M_3^2 \pi_3}{F_5} + \ldots \quad (D.2)$$

into the effective interaction Lagrangian

$$L_{N_{1535} N} = \bar{h}_{N_{1535} N} \chi_{-} N + h.c. \quad (D.3)$$

Footnote 5: The proportionality of $g_1^a$ to $3b_F - b_D$ may come at first sight as a surprise. Note, however, that the strange-quark content of the nucleon is proportional to $b_b + b_d - b_F$ to leading order in the chiral expansion, such that $g_1^a$ for small or vanishing $y$ is factually proportional to $2 b_b + b_d - b_F$ which in turn is proportional to $2 c_5$. For more details see e.g. ref. [34,24].

Footnote 6: In fact, the latter equation which is based on eq. (5.7) of ref. [24] predicts that the NLO correction to $c_5$ is much larger than $c_5$ (or $b_D + b_F$) itself, namely $\Delta c_5 = 0.49$ GeV$^{-1}$. This quantity is of similar size as $\Delta c_5 = +0.2$ GeV$^{-1}$. 
the second vertex by the decay of the resonance into a $\eta$ and a nucleon, followed by $\eta$ $\rightarrow \pi^0$ mixing (black circle). Note that the second topology of the diagram where the pion emission comes first is included in the calculation.

we get

$$L_{N1535N} = hN_{1535}^\dagger \left(-M_\pi^2(1-\epsilon^2)\vec{\theta} + \frac{2M_\pi^2}{F_\pi} \right) N + h.c.$$  

(D.4)

The first term provides the CP-odd transition of a nucleon into the $N^\ast$. As illustrated in fig. 6 we may model the second vertex by the decay of the resonance into an $\eta$ and a nucleon, followed by $\eta$ $\rightarrow \pi^0$ mixing; using the leading order ChPT expression for the mixing amplitude

$$\epsilon_{\pi^0\eta} \approx \sqrt{\frac{3}{4}} \frac{B(m_d-m_u)}{M_\eta^2-M_\pi^2} \approx 1.37\%,$$  

(D.5)

we can express $h$ by $g^*$ and $\epsilon_{\pi^0\eta}$ as

$$\tilde{h} = \epsilon_{\pi^0\eta} \frac{g^*}{2\epsilon M_\pi^2}.$$  

(D.6)

Thus the interaction Lagrangian (D.4) can be rewritten as

$$L_{N\cdot N_{\chi^\ast}} = g^* \epsilon_{\pi^0\eta} \left(\frac{F_\pi(1-\epsilon^2)}{-2\epsilon} + \pi_3 \right) N_{1535}^\ast N + h.c.$$  

(D.7)

In summary, we get the following estimate for the odd-parity contribution to the CP-violating isospin-breaking $\pi NN$ coupling constant

$$\delta g_1^\theta = |g^*|^2(\epsilon_{\pi^0\eta})^2 \frac{F_\pi(1-\epsilon^2)}{m_{N_{1535}}-m_N} \approx (0.6 \pm 0.3) \cdot 10^{-3} \tilde{\theta},$$  

(D.8)

which is only one third of the NDA estimate

$$|\epsilon| \approx \frac{M_\eta^4}{m_N F_\pi} \tilde{\theta} \approx 1.7 \cdot 10^{-3} \tilde{\theta}.$$

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