

6-16-2011

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Publication Info

Published in *Physical Review C*, Volume 83, Issue 6, 2011, pages 065503-1-065503-7.

Song, Y.-H., Lazauskas, R., and Gudkov, V. (2011). Time reversal invariance violation in neutron-deuteron scattering. *Physical Review C*, 83(6), 065503-1 - 065503-7. doi: 10.1103/PhysRevC.83.065503

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Time reversal invariance violation in neutron-deuteron scattering

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(Received 14 April 2011; published 16 June 2011)

Time reversal invariance-violating (TRIV) effects in low-energy elastic neutron-deuteron scattering are calculated using meson exchange and EFT-type TRIV potentials in a distorted-wave Born approximation with realistic hadronic strong interaction wave functions, obtained by solving the three-body Faddeev equations in configuration space. The relation between TRIV and parity-violating observables is discussed.

DOI: [10.1103/PhysRevC.83.065503](https://doi.org/10.1103/PhysRevC.83.065503)

PACS number(s): 24.80.+y, 25.10.+s, 11.30.Er, 13.75.Cs

I. INTRODUCTION

The search for time reversal invariance violation (TRIV) in nuclear physics has been a subject of experimental and theoretical investigation for several decades. The search has covered a large variety of nuclear reactions and nuclear decays with T -violating parameters, which are sensitive to either CP -odd and P -odd (or T - and P -violating) interactions or T -violating P -conserving (C -odd and P -even) interactions. There are a number of advantages to searching for TRIV in nuclear processes. The main advantage is the possibility of an enhancement of T -violating observables by many orders of magnitude due to complex nuclear structures (see, for example, Ref. [1] and references therein). Another advantage is the availability of many systems with T -violating parameters. This provides assurance that there will be enough observations to avoid a possible “accidental” cancellation of T -violating effects due to unknown structural factors related to the strong interactions. Taking into account that different models of CP violation may contribute differently to a particular T/CP observable,¹ which may have unknown theoretical uncertainties, TRIV nuclear processes should provide complementary information to electric dipole moment (EDM) measurements.

One promising approach to searching for TRIV in nuclear reactions is a measurement of TRIV effects in the transmission of polarized neutrons through a polarized target. These effects could be measured at new spallation neutron facilities, such as the SNS at the Oak Ridge National Laboratory or the J-SNS at J-PARC in Japan. It was shown that these TRIV effects can be enhanced [2] by a factor of 10^6 . Similar enhancement factors have been observed for parity-violating effects in neutron scattering. In contrast to the parity-violating (PV) case, the enhancement of TRIV effects leads not only to an

opportunity to observe T violation, but also to validate models of CP violation based on the values of observed parameters. However, existing estimates of CP -violating effects in nuclear reactions have, at most, an order of magnitude of accuracy. In this relation, it is interesting to compare the calculation of TRIV effects in complex nuclei with the calculations of these effects in the simplest few-body systems, which could be useful for clarification of the influence of nuclear structure on TRIV effects. Therefore, as a first step to the investigation of many-body nuclear effects, we study TRIV and parity-violating effects in one of the simplest available nuclear process, namely, elastic neutron-deuteron scattering.

We treat TRIV nucleon-nucleon interactions as a perturbation, while unperturbed three-body wave functions are obtained by solving Faddeev equations for a realistic strong interaction Hamiltonian, based on the AV18 + UIX interaction model. To describe the TRIV potentials, we use both a meson-exchange model and the effective field theory (EFT) approach.

II. OBSERVABLES

We consider TRIV and PV effects related to the $\sigma_n \cdot (\mathbf{p} \times \mathbf{I})$ correlation, where σ_n is the neutron spin, \mathbf{I} is the target spin, and \mathbf{p} is the neutron momentum, which can be observed in the transmission of polarized neutrons through a target with polarized nuclei. This correlation leads to a difference [3] between the total neutron cross sections for σ_n parallel and antiparallel to $\mathbf{p} \times \mathbf{I}$,

$$\Delta\sigma_{TP} = \frac{4\pi}{p} \text{Im}(f_+ - f_-), \quad (1)$$

and to neutron spin rotation angle [4] ϕ around the axis $\mathbf{p} \times \mathbf{I}$,

$$\frac{d\phi_{TP}}{dz} = -\frac{2\pi N}{p} \text{Re}(f_+ - f_-). \quad (2)$$

Here, $f_{+,-}$ are the zero-angle scattering amplitudes for neutrons polarized parallel and antiparallel to the $\mathbf{p} \times \mathbf{I}$ axis, respectively, z is the target length, and N is the number of target nuclei per unit volume. It should be noted that these two parameters can not be simulated by final-state interactions (see, for example, [1] and references therein),

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¹For example, the QCD θ term can contribute to neutron EDM, but can not be observed in K^0 -meson decays. On the other hand, the CP -odd phase of the Cabibbo-Kobayashi-Maskawa matrix was measured in K^0 -meson decays, but its contribution to the neutron EDM is extremely small and beyond the reach of current experimental precision.

therefore, measurements of them are unambiguous tests of violation of time reversal invariance, similar to the case of the neutron electric dipole moment.

The scattering amplitudes can be represented in terms of the matrix \hat{R} , which is related to the scattering matrix \hat{S} as $\hat{R} = \hat{1} - \hat{S}$. We define the matrix element $R_{l'S',lS}^J = \langle l'S' | R^J | lS \rangle$, where unprimed and primed parameters correspond to initial and final states, l is an orbital angular momentum between neutron and deuteron, S is a sum of neutron spin and deuteron total angular momentum, and J is the total angular momentum of the neutron-deuteron system. For low-energy neutron scattering, one can consider only s - and p -wave contributions, which lead to the following expressions for the TRIV parameters:

$$\frac{1}{N} \frac{d\phi_{\mathcal{T}P}}{dz} = -\frac{\pi}{2p^2} \text{Re} \left[\sqrt{2} R_{0\frac{1}{2},1\frac{3}{2}}^{\frac{1}{2}} - \sqrt{2} R_{1\frac{1}{2},0\frac{3}{2}}^{\frac{1}{2}} + 2R_{0\frac{3}{2},1\frac{1}{2}}^{\frac{3}{2}} - 2R_{1\frac{3}{2},0\frac{1}{2}}^{\frac{3}{2}} \right], \quad (3)$$

$$\Delta\sigma_{\mathcal{T}P} = \frac{\pi}{p^2} \text{Im} \left[\sqrt{2} R_{0\frac{1}{2},1\frac{3}{2}}^{\frac{1}{2}} - \sqrt{2} R_{1\frac{1}{2},0\frac{3}{2}}^{\frac{1}{2}} + 2R_{0\frac{3}{2},1\frac{1}{2}}^{\frac{3}{2}} - 2R_{1\frac{3}{2},0\frac{1}{2}}^{\frac{3}{2}} \right]. \quad (4)$$

The symmetry-violating \hat{R} -matrix elements can be calculated with a high level of accuracy in the distorted-wave Born approximation (DWBA) as

$$R_{l'S',lS}^J \simeq 4i^{-l'+l+1} \mu p^{(-)} \langle \Psi, (l'S') J J^z | V_{\mathcal{T}P} | \Psi, (lS) J J^z \rangle^{(+)}, \quad (5)$$

where μ is a neutron-deuteron reduced mass, $V_{\mathcal{T}P}$ is TRIV nucleon-nucleon potential, and $|\Psi, (l'S') J J^z \rangle^{(\pm)}$ are solutions of three-body Faddeev equations in configuration space for a strong interaction Hamiltonian satisfying outgoing (incoming) boundary conditions. The factor $i^{-l'+l}$ in this expression is introduced to match the R -matrix definition in the modified spherical harmonics convention [5], with the wave functions in the spherical harmonics convention used for wave-function calculations. The matrix elements of the TRIV potential in the spherical harmonics convention are symmetric, and the R matrix in modified spherical harmonics convention is antisymmetric under the exchange between initial and final states.

For calculations of wave functions, we used a jj -coupling scheme instead of a lS coupling scheme. We can relate R -matrix elements in the lS coupling scheme to those in the jj -coupling scheme using a unitary transformation (see, for example, [6])

$$|l_y \otimes (s_k \otimes j_x)_S \rangle_{J J_z} = \sum_{j_y} |j_x \otimes (l_y \otimes s_k)_{j_y} \rangle_{J J_z} \times (-1)^{j_x+j_y-J} (-1)^{l_y+s_k+j_x+J} \times [(2j_y+1)(2S+1)]^{\frac{1}{2}} \begin{Bmatrix} l_y & s_k & j_y \\ j_x & J & S \end{Bmatrix}. \quad (6)$$

Then,

$$R_{1\frac{3}{2},0\frac{1}{2}}^{\frac{1}{2}} = \frac{2\sqrt{2}}{3} \mathcal{R}_{1\frac{1}{2},0\frac{1}{2}}^{\frac{1}{2}} - \frac{1}{3} \mathcal{R}_{1\frac{3}{2},0\frac{1}{2}}^{\frac{1}{2}}, \\ R_{1\frac{1}{2},0\frac{3}{2}}^{\frac{3}{2}} = R_{1\frac{3}{2},0\frac{3}{2}}^{\frac{3}{2}} = -\frac{2}{3} \mathcal{R}_{1\frac{1}{2},0\frac{1}{2}}^{\frac{3}{2}} - \frac{\sqrt{5}}{3} \mathcal{R}_{1\frac{3}{2},0\frac{1}{2}}^{\frac{3}{2}} \quad (7)$$

where $\mathcal{R}_{l'j',lj}^J$ is an R matrix in the jj basis.

III. TIME REVERSAL VIOLATING POTENTIALS

The most general form for the time reversal violating and parity-violating part of the nucleon-nucleon Hamiltonian up to first order in the relative nucleon momentum can be written as the sum of momentum-independent and momentum-dependent parts $H^{\mathcal{T}P} = H_{\text{stat}}^{\mathcal{T}P} + H_{\text{nonstatic}}^{\mathcal{T}P}$ [7]:

$$H_{\text{stat}}^{\mathcal{T}P} = g_1(r) \boldsymbol{\sigma}_- \cdot \hat{r} + g_2(r) \tau_1 \cdot \tau_2 \boldsymbol{\sigma}_- \cdot \hat{r} + g_3(r) T_{12}^z \boldsymbol{\sigma}_- \cdot \hat{r} + g_4(r) \tau_+ \boldsymbol{\sigma}_- \cdot \hat{r} + g_5(r) \tau_- \boldsymbol{\sigma}_+ \cdot \hat{r}, \quad (8)$$

$$H_{\text{nonstatic}}^{\mathcal{T}P} = [g_6(r) + g_7(r) \tau_1 \cdot \tau_2 + g_8(r) T_{12}^z + g_9(r) \tau_+] \boldsymbol{\sigma}_\times \cdot \frac{\bar{\mathbf{p}}}{m_N} + [g_{10}(r) + g_{11}(r) \tau_1 \cdot \tau_2 + g_{12}(r) T_{12}^z + g_{13}(r) \tau_+] \times \left(\hat{r} \cdot \boldsymbol{\sigma}_\times \hat{r} \cdot \frac{\bar{\mathbf{p}}}{m_N} - \frac{1}{3} \boldsymbol{\sigma}_\times \cdot \frac{\bar{\mathbf{p}}}{m_N} \right) + g_{14}(r) \tau_- \left[\hat{r} \cdot \boldsymbol{\sigma}_1 \hat{r} \cdot \left(\boldsymbol{\sigma}_2 \times \frac{\bar{\mathbf{p}}}{m_N} \right) + \hat{r} \cdot \boldsymbol{\sigma}_2 \hat{r} \cdot \left(\boldsymbol{\sigma}_1 \times \frac{\bar{\mathbf{p}}}{m_N} \right) \right] + g_{15}(r) (\tau_1 \times \tau_2)^z \boldsymbol{\sigma}_+ \cdot \frac{\bar{\mathbf{p}}}{m_N} + g_{16}(r) (\tau_1 \times \tau_2)^z \left(\hat{r} \cdot \boldsymbol{\sigma}_+ \hat{r} \cdot \frac{\bar{\mathbf{p}}}{m_N} - \frac{1}{3} \boldsymbol{\sigma}_+ \cdot \frac{\bar{\mathbf{p}}}{m_N} \right), \quad (9)$$

where $\vec{\sigma}_\pm = (\vec{\sigma}_1 \pm \vec{\sigma}_2)$, $\vec{\sigma}_\times = (\vec{\sigma}_1 \times \vec{\sigma}_2)$, $\vec{r} = \vec{r}_1 - \vec{r}_2$, and the exact form of $g_i(r)$ depends on the details of particular theory. Here, we consider three different approaches for the description of TRIV interactions: a meson-exchange model, pionless EFT, and pionful EFT.

The TRIV meson-exchange potential, in general, involves exchanges of pions ($J^P = 0^-, m_\pi = 140$ MeV), η mesons ($J^P = 0^-, m_\eta = 550$ MeV), and ρ and ω mesons ($J^P = 1^-, m_{\rho,\omega} = 770$ and 780 MeV). To derive this potential, we use the strong \mathcal{L}^{st} and TRIV $\mathcal{L}_{\mathcal{T}P}$ Lagrangians, which can be written as [8,9]

$$\mathcal{L}^{st} = g_\pi \bar{N} i \gamma_5 \tau^a \pi^a N + g_\eta \bar{N} i \gamma_5 \eta N - g_\rho \bar{N} \left(\gamma^\mu - i \frac{\chi_V}{2m_N} \sigma^{\mu\nu} q_\nu \right) \tau^a \rho_\mu^a N - g_\omega \bar{N} \left(\gamma^\mu - i \frac{\chi_S}{2m_N} \sigma^{\mu\nu} q_\nu \right) \omega_\mu N, \quad (10)$$

$$\begin{aligned}
\mathcal{L}_{\mathcal{T}P} = & \bar{N} [\bar{g}_\pi^{(0)} \tau^a \pi^a + \bar{g}_\pi^{(1)} \pi^0 + \bar{g}_\pi^{(2)} (3\tau^z \pi^0 - \tau^a \pi^a)] N \\
& + \bar{N} [\bar{g}_\eta^{(0)} \eta + \bar{g}_\eta^{(1)} \tau^z \eta] N \\
& + \bar{N} \frac{1}{2m_N} [\bar{g}_\rho^{(0)} \tau^a \rho_\mu^a + \bar{g}_\rho^{(1)} \rho_\mu^0 + \bar{g}^{(2)} \\
& \times (3\tau^z \rho_\mu^0 - \tau^a \rho_\mu^a)] \sigma^{\mu\nu} q_\nu \gamma_5 N \\
& + \bar{N} \frac{1}{2m_N} [\bar{g}_\omega^{(0)} \omega_\mu + \bar{g}_\omega^{(1)} \tau^z \omega_\mu] \sigma^{\mu\nu} q_\nu \gamma_5 N, \quad (11)
\end{aligned}$$

where $q_\nu = p_\nu - p'_\nu$, χ_V and χ_S are isovector and scalar magnetic moments of a nucleon ($\chi_V = 3.70$ and $\chi_S = -0.12$), and $\bar{g}_\alpha^{(i)}$ are TRIV meson-nucleon coupling constants. Further, we use the following values for strong-coupling constants: $g_\pi = 13.07$, $g_\eta = 2.24$, $g_\rho = 2.75$, and $g_\omega = 8.25$.

The meson-exchange models from these Lagrangians lead to a TRIV potential

$$\begin{aligned}
V_{\mathcal{T}P} = & \left[-\frac{\bar{g}_\eta^{(0)} g_\eta m_\eta^2}{2m_N 4\pi} Y_1(x_\eta) + \frac{\bar{g}_\omega^{(0)} g_\omega m_\omega^2}{2m_N 4\pi} Y_1(x_\omega) \right] \boldsymbol{\sigma}_- \cdot \hat{r} \\
& + \left[-\frac{\bar{g}_\pi^{(0)} g_\pi m_\pi^2}{2m_N 4\pi} Y_1(x_\pi) + \frac{\bar{g}_\rho^{(0)} g_\rho m_\rho^2}{2m_N 4\pi} Y_1(x_\rho) \right] \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \boldsymbol{\sigma}_- \cdot \hat{r} \\
& + \left[-\frac{\bar{g}_\pi^{(2)} g_\pi m_\pi^2}{2m_N 4\pi} Y_1(x_\pi) + \frac{\bar{g}_\rho^{(2)} g_\rho m_\rho^2}{2m_N 4\pi} Y_1(x_\rho) \right] T_{12}^z \boldsymbol{\sigma}_- \cdot \hat{r} \\
& + \left[-\frac{\bar{g}_\pi^{(1)} g_\pi m_\pi^2}{4m_N 4\pi} Y_1(x_\pi) + \frac{\bar{g}_\eta^{(1)} g_\eta m_\eta^2}{4m_N 4\pi} Y_1(x_\eta) \right. \\
& \left. + \frac{\bar{g}_\rho^{(1)} g_\rho m_\rho^2}{4m_N 4\pi} Y_1(x_\rho) + \frac{\bar{g}_\omega^{(1)} g_\omega m_\omega^2}{2m_N 4\pi} Y_1(x_\omega) \right] \boldsymbol{\tau}_+ \boldsymbol{\sigma}_- \cdot \hat{r} \\
& + \left[-\frac{\bar{g}_\pi^{(1)} g_\pi m_\pi^2}{4m_N 4\pi} Y_1(x_\pi) - \frac{\bar{g}_\eta^{(1)} g_\eta m_\eta^2}{4m_N 4\pi} Y_1(x_\eta) \right. \\
& \left. - \frac{\bar{g}_\rho^{(1)} g_\rho m_\rho^2}{4m_N 4\pi} Y_1(x_\rho) + \frac{\bar{g}_\omega^{(1)} g_\omega m_\omega^2}{2m_N 4\pi} Y_1(x_\omega) \right] \boldsymbol{\tau}_- \boldsymbol{\sigma}_+ \cdot \hat{r}, \quad (12)
\end{aligned}$$

where $T_{12}^z = 3\tau_1^z \tau_2^z - \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$, $Y_1(x) = (1 + \frac{1}{x}) \frac{e^{-x}}{x}$, and $x_a = m_a r$.

By comparing Eq. (8) with this potential, one can see that the $g_i(r)$ functions in the meson-exchange model are defined as

$$\begin{aligned}
g_1^{ME}(r) &= -\frac{\bar{g}_\eta^{(0)} g_\eta m_\eta^2}{2m_N 4\pi} Y_1(x_\eta) + \frac{\bar{g}_\omega^{(0)} g_\omega m_\omega^2}{2m_N 4\pi} Y_1(x_\omega), \\
g_2^{ME}(r) &= -\frac{\bar{g}_\pi^{(0)} g_\pi m_\pi^2}{2m_N 4\pi} Y_1(x_\pi) + \frac{\bar{g}_\rho^{(0)} g_\rho m_\rho^2}{2m_N 4\pi} Y_1(x_\rho), \\
g_3^{ME}(r) &= -\frac{\bar{g}_\pi^{(2)} g_\pi m_\pi^2}{2m_N 4\pi} Y_1(x_\pi) + \frac{\bar{g}_\rho^{(2)} g_\rho m_\rho^2}{2m_N 4\pi} Y_1(x_\rho), \\
g_4^{ME}(r) &= -\frac{\bar{g}_\pi^{(1)} g_\pi m_\pi^2}{4m_N 4\pi} Y_1(x_\pi) + \frac{\bar{g}_\eta^{(1)} g_\eta m_\eta^2}{4m_N 4\pi} Y_1(x_\eta) \\
&+ \frac{\bar{g}_\rho^{(1)} g_\rho m_\rho^2}{4m_N 4\pi} Y_1(x_\rho) + \frac{\bar{g}_\omega^{(1)} g_\omega m_\omega^2}{2m_N 4\pi} Y_1(x_\omega)
\end{aligned}$$

$$\begin{aligned}
g_5^{ME}(r) &= -\frac{\bar{g}_\pi^{(1)} g_\pi m_\pi^2}{4m_N 4\pi} Y_1(x_\pi) - \frac{\bar{g}_\eta^{(1)} g_\eta m_\eta^2}{4m_N 4\pi} Y_1(x_\eta) \\
&- \frac{\bar{g}_\rho^{(1)} g_\rho m_\rho^2}{4m_N 4\pi} Y_1(x_\rho) + \frac{\bar{g}_\omega^{(1)} g_\omega m_\omega^2}{2m_N 4\pi} Y_1(x_\omega). \quad (13)
\end{aligned}$$

For the TRIV potentials in the pionless EFT potential, these functions are

$$\begin{aligned}
g_1^\pi(r) &= \frac{c_1^\pi}{2m_N} \frac{d}{dr} \delta^{(3)}(\mathbf{r}) \rightarrow -\frac{c_1^\pi \mu^2}{2m_N 4\pi} Y_1(\mu r), \\
g_2^\pi(r) &= \frac{c_2^\pi}{2m_N} \frac{d}{dr} \delta^{(3)}(\mathbf{r}) \rightarrow -\frac{c_2^\pi \mu^2}{2m_N 4\pi} Y_1(\mu r), \\
g_3^\pi(r) &= \frac{c_3^\pi}{2m_N} \frac{d}{dr} \delta^{(3)}(\mathbf{r}) \rightarrow -\frac{c_3^\pi \mu^2}{2m_N 4\pi} Y_1(\mu r), \\
g_4^\pi(r) &= \frac{c_4^\pi}{2m_N} \frac{d}{dr} \delta^{(3)}(\mathbf{r}) \rightarrow -\frac{c_4^\pi \mu^2}{2m_N 4\pi} Y_1(\mu r), \\
g_5^\pi(r) &= \frac{c_5^\pi}{2m_N} \frac{d}{dr} \delta^{(3)}(\mathbf{r}) \rightarrow -\frac{c_5^\pi \mu^2}{2m_N 4\pi} Y_1(\mu r), \quad (14)
\end{aligned}$$

where the low-energy constants (LECs) c_i^π of the pionless EFT have the dimension [fm²]. In our calculations with this potential, we use the Yukawa function [$\frac{\mu^3}{4\pi} Y_0(\mu r)$, where $Y_0(x) = \frac{e^{-x}}{x}$] with the regularization scale $\mu = m_\pi$, instead of the singular $\delta^{(3)}(r)$ in Ref. [9].

The pionful EFT acquires long-range terms due to the one-pion exchange in addition to the short-range-term expressions equivalent to those provided by the pionless EFT. Then, by ignoring two-pion-exchange contributions at the middle range and higher-order corrections, one can write the $g_i(r)$ functions for the pionful EFT as

$$\begin{aligned}
g_1^\pi(r) &= -\frac{c_1^\pi \mu^2}{2m_N 4\pi} Y_1(\mu r), \\
g_2^\pi(r) &= -\frac{c_2^\pi \mu^2}{2m_N 4\pi} Y_1(\mu r) - \frac{\bar{g}_\pi^{(0)} g_\pi m_\pi^2}{2m_N 4\pi} Y_1(x_\pi), \\
g_3^\pi(r) &= -\frac{c_3^\pi \mu^2}{2m_N 4\pi} Y_1(\mu r) - \frac{\bar{g}_\pi^{(2)} g_\pi m_\pi^2}{2m_N 4\pi} Y_1(x_\pi), \\
g_4^\pi(r) &= -\frac{c_4^\pi \mu^2}{2m_N 4\pi} Y_1(\mu r) - \frac{\bar{g}_\pi^{(1)} g_\pi m_\pi^2}{4m_N 4\pi} Y_1(x_\pi), \\
g_5^\pi(r) &= -\frac{c_5^\pi \mu^2}{2m_N 4\pi} Y_1(\mu r) - \frac{\bar{g}_\pi^{(1)} g_\pi m_\pi^2}{4m_N 4\pi} Y_1(x_\pi). \quad (15)
\end{aligned}$$

For this potential, the cutoff scale μ is larger than the pion mass because the pion is a degree of freedom of the theory. Therefore, in general, the magnitudes of LECs and their scaling behaviors, as a function of a cutoff parameter $c_i^\pi(\mu)$, are different from the $c_i^\pi(\mu)$ scaling behaviors.

One can see that all three potentials, which come from different approaches, have exactly the same operator structure. The only difference between them is related to the different scalar functions multiplying each operator. These, in turn, differ only through the presence of different characteristic masses: m_π , m_η , m_ρ , and m_ω . Therefore, to unify notations, it is convenient to define new constants C_n^a (of dimension [fm]) and

the scalar function $f_n^a(r) = \frac{\mu^2}{4\pi} Y_1(\mu r)$ (of dimension $[\text{fm}^{-2}]$) as

$$g_n(r) \equiv \sum_a C_n^a f_n^a(r), \quad (16)$$

where the form of C_n^a and $f_n^a(r)$ can be read from Eqs. (13), (14), and (15).

Since nonstatic TRIV potentials, with $g_{n>5}$, do not appear either in the meson-exchange model or in the lowest-order EFTs, they can be considered as higher-order corrections to the lowest-order EFT or related to heavy-meson contributions in the meson-exchange model. Nevertheless, for completeness, we estimate the contributions of these operators using $f_n^a(r)$ functions with proper mass scales.

IV. CALCULATION OF TRIV AMPLITUDES

The nonperturbed (parity-conserving) three-body wave functions for neutron-deuteron scattering are obtained by solving Faddeev equations (also often called Kowalski-Noyes equations) in configuration space [10,11]. The wave function in the Faddeev formalism is a sum of three Faddeev components

$$\Psi(\mathbf{x}, \mathbf{y}) = \psi_1(\mathbf{x}_1, \mathbf{y}_1) + \psi_2(\mathbf{x}_2, \mathbf{y}_2) + \psi_3(\mathbf{x}_3, \mathbf{y}_3). \quad (17)$$

In the particular case of three identical particles (this becomes formally true for the three-nucleon system in the isospin formalism), the three Faddeev equations (components) become formally identical. In terms of the three-nucleon force, which under the nucleon permutation might be expressed as a symmetric sum of three terms $V_{ijk} = V_{ij}^k + V_{jk}^i + V_{ki}^j$, the Faddeev equations read as

$$(E - H_0 - V_{ij})\psi_k = V_{ij}(\psi_i + \psi_j) + \frac{1}{2}(V_{jk}^i + V_{ki}^j)\Psi, \quad (18)$$

where (ijk) are the particle indices, H_0 is the kinetic energy operator, V_{ij} is the two-body force between particles i and j , and $\psi_k = \psi_{ij,k}$ is the Faddeev component.

By using relative Jacobi coordinates $\mathbf{x}_k = (\mathbf{r}_j - \mathbf{r}_i)$ and $\mathbf{y}_k = \frac{2}{\sqrt{3}}(\mathbf{r}_k - \frac{\mathbf{r}_i + \mathbf{r}_j}{2})$, one can expand these Faddeev components in a bipolar harmonic basis:

$$\psi_k = \sum_{\alpha} \frac{F_{\alpha}(x_k, y_k)}{x_k y_k} [l_x(s_i s_j)_{s_x}]_{j_x} (l_y s_k)_{j_y} \rangle_{JM} \otimes |(t_i t_j)_{t_x} t_k \rangle_{TT_z}, \quad (19)$$

where the index α represents all allowed combinations of the quantum numbers present in the brackets, l_x and l_y are the partial angular momenta associated with respective Jacobi coordinates, and s_i and t_i are the spins and isospins of the individual particles. The functions $F_{\alpha}(x_k, y_k)$ are called partial Faddeev amplitudes. It should be noted that the total angular momentum J as well as its projection M are conserved, but the total isospin T of the system is not conserved due to the presence of charge-dependent terms in nuclear interactions.

Boundary conditions for Eq. (18) can be written in Dirichlet form. Thus, the partial Faddeev amplitudes satisfy the regularity conditions

$$F_{\alpha}(0, y_k) = F_{\alpha}(x_k, 0) = 0. \quad (20)$$

For neutron-deuteron scattering with energies below the breakup threshold, the Faddeev components vanish for $\mathbf{x}_k \rightarrow \infty$. If $\mathbf{y}_k \rightarrow \infty$, then interactions between the particle k and the cluster ij are negligible, and the Faddeev components ψ_i and ψ_j vanish. Then, for the component ψ_k , which describes the plane wave of the particle k with respect to the bound particle pair ij ,

$$\begin{aligned} \lim_{y_k \rightarrow \infty} \psi_k(\mathbf{x}_k, \mathbf{y}_k)_{l_n j_n} &= \frac{1}{\sqrt{3}} \sum_{j_n' l_n'} |\{\phi_d(\mathbf{x}_k)\}_{j_d} \otimes \{Y_{l_n'}(\hat{\mathbf{y}}_k) \otimes s_k\}_{j_n'} \rangle_{JM} \otimes |(t_i t_j)_{t_d} t_k \rangle_{\frac{1}{2}, -\frac{1}{2}} \\ &\times \frac{i}{2} [\delta_{l_n' j_n', l_n j_n} h_{l_n'}^-(pr_{nd}) - S_{l_n' j_n', l_n j_n} h_{l_n'}^+(pr_{nd})], \end{aligned} \quad (21)$$

where the deuteron, being formed from nucleons i and j , has quantum numbers $s_d = 1$, $j_d = 1$, and $t_d = 0$, and its wave function $\phi_d(\mathbf{x}_k)$ is normalized to unity. Here, $r_{nd} = (\sqrt{3}/2)y_k$ is the relative distance between the neutron and the deuteron target, and $h_{l_n}^{\pm}$ are the spherical Hankel functions. The expression (21) is normalized to satisfy a condition of unit flux for the nd scattering wave function.

By using a decomposition of the momentum $\bar{\mathbf{p}}$, which acts only on the nuclear wave function

$$\bar{\mathbf{p}} = \frac{i \overleftarrow{\nabla}_x - i \overrightarrow{\nabla}_x}{2} = \frac{i \hat{x}}{2} \left(\frac{\overleftarrow{\partial}}{\partial x} - \frac{\overrightarrow{\partial}}{\partial x} \right) + \frac{i}{2x} \left(\overleftarrow{\nabla}_{\Omega} - i \overrightarrow{\nabla}_{\Omega} \right), \quad (22)$$

we can represent general matrix elements of local two-body parity-violating potential operators as

$$\begin{aligned} {}^{(-)}\langle \Psi_f | O | \Psi_i \rangle^{(+)} &= \left(\frac{\sqrt{3}}{2} \right)^3 \sum_{\alpha\beta} \left[\int dx x^2 dy y^2 \right. \\ &\times \left(\frac{\tilde{F}_{f,\alpha}^{(+)}(x, y)}{xy} \right) \hat{X}(x) \left(\frac{\tilde{F}_{i,\beta}^{(+)}(x, y)}{xy} \right) \Big] \\ &\times \langle \alpha | \hat{O}(\hat{x}) | \beta \rangle, \end{aligned} \quad (23)$$

where (\pm) means outgoing and incoming boundary conditions, and $\hat{X}(x)$ is a scalar function or a derivative with respect to x acting on the wave function. [Note that we have used the fact that $(\tilde{F}^{(-)})^* = \tilde{F}^{(+)}$.] The partial amplitudes $\tilde{F}_{i(f),\alpha}(x, y)$ represent the total system's wave function in one selected basis set among three possible angular momentum coupling sequences for three particle angular momenta:

$$\begin{aligned} \Psi_{i(f)}(x, y) &= \sum_{\alpha} \frac{\tilde{F}_{i(f),\alpha}(x, y)}{xy} [l_x(s_i s_j)_{s_x}]_{j_x} (l_y s_k)_{j_y} \rangle_{JM} \\ &\otimes |(t_i t_j)_{t_x} t_k \rangle_{TT_z}. \end{aligned} \quad (24)$$

TABLE I. Typical matrix elements of the TRIV potential $\text{Re} \frac{\langle (l_y j_y), J | V_{np}^{TP} | (l_y j_y), J \rangle}{\bar{C}_{np}}$ in the jj -coupling scheme with the AV18 + UIX strong potential in the zero-energy limit. The imaginary part of the matrix element is zero in the zero-energy limit. Scalar functions are chosen as $\frac{m_\pi^2}{4\pi} Y_1(m_\pi r)$ for operators 1–5 and $\frac{m_\pi^2}{4\pi} Y_0(m_\pi r)$ for operators 6–16. $O_{3,8,12} = 0$ because of isospin selection rules. All numbers are in units of fm^2 .

n	$\langle 1 \frac{1}{2} v^{1/2} 0 \frac{1}{2} \rangle / p$	$\langle 1 \frac{3}{2} v^{1/2} 0 \frac{1}{2} \rangle / p$	$\langle 1 \frac{1}{2} v^{3/2} 0 \frac{1}{2} \rangle / p$	$\langle 1 \frac{3}{2} v^{3/2} 0 \frac{1}{2} \rangle / p$
1	0.590×10^{-01}	-0.787×10^{-01}	0.151×10^{-01}	0.177×10^{-01}
2	$0.627 \times 10^{+00}$	-0.863×10^{-01}	$-0.144 \times 10^{+00}$	$-0.167 \times 10^{+00}$
4	$-0.268 \times 10^{+00}$	$0.107 \times 10^{+00}$	0.330×10^{-01}	0.379×10^{-01}
5	$0.321 \times 10^{+00}$	$-0.267 \times 10^{+00}$	$-0.199 \times 10^{+00}$	-0.691×10^{-01}
6	0.719×10^{-01}	-0.104×10^{-01}	-0.115×10^{-01}	-0.141×10^{-01}
7	-0.206×10^{-01}	0.520×10^{-02}	0.337×10^{-01}	0.384×10^{-01}
9	-0.650×10^{-01}	0.865×10^{-02}	0.238×10^{-03}	0.134×10^{-02}
10	0.106×10^{-01}	-0.932×10^{-03}	0.658×10^{-03}	0.622×10^{-03}
11	0.171×10^{-01}	-0.548×10^{-03}	-0.237×10^{-02}	-0.273×10^{-02}
13	-0.163×10^{-01}	0.111×10^{-02}	0.131×10^{-03}	0.288×10^{-03}
14	0.649×10^{-02}	-0.628×10^{-02}	-0.876×10^{-02}	-0.250×10^{-03}
15	0.338×10^{-01}	-0.230×10^{-01}	-0.293×10^{-01}	-0.198×10^{-02}
16	0.128×10^{-01}	-0.816×10^{-02}	-0.119×10^{-01}	-0.335×10^{-03}

The “angular” part of the matrix element is

$$\langle \alpha | \hat{O}(\hat{x}) | \beta \rangle \equiv \int d\hat{x} \int d\hat{y} \mathcal{Y}_\alpha^\dagger(\hat{x}, \hat{y}) \hat{O}(\hat{x}) \mathcal{Y}_\beta(\hat{x}, \hat{y}), \quad (25)$$

where $\mathcal{Y}_\alpha(\hat{x}, \hat{y})$ is a tensor bipolar spherical harmonic with a quantum number α . One can see that the operators for “angular” matrix elements have the following structure:

$$\hat{O}(\hat{x}) = (\tau_i \odot \tau_j)(\sigma_i \odot \sigma_j) \cdot (\hat{x}, \text{ or } \overleftarrow{\nabla}_\Omega, \text{ or } \overrightarrow{\nabla}_\Omega), \quad (26)$$

where $\odot, \otimes = \pm, \times$. We calculated the “angular” matrix elements by representing all operators as a tensor product of isospin, spin, and spatial operators. For details of the calculations of matrix elements, see Ref. [6]. Similar approaches have been successfully applied for the calculations of weak and electromagnetic processes involving three- and four-body hadronic systems [12–17] and for the calculation of parity-violating effects in neutron-deuteron scattering [6, 18].

V. RESULTS AND DISCUSSIONS

Typical results for the contributions of different operators in a TRIV potential to matrix elements are shown in Table I, where the mass scale was chosen to be equal to $\mu = 138 \text{ MeV}$. As was discussed, both the pionless and the pionful EFTs in the leading order, as well as the meson-exchange model, have only five operators that have nonzero coefficients. Taking into account that the characteristic mass scale μ for operators with $g_{n \geq 6}$ should be at least larger than twice the pion mass, the actual contributions of these operators are at least one order of magnitude smaller than the values shown in Table I. Thus, one can neglect contributions from the suppressed $n \geq 6$ operators provided that the coupling constants satisfy the naturalness assumption.

The possible contributions of different mesons to the TRIV amplitude at $E_{cm} = 100 \text{ keV}$ are summarized in Table II. Using these data, the observable parameters at the neutron energy

$E_{cm} = 100 \text{ keV}$ can be rewritten in terms of TRIV meson coupling constants as

$$\begin{aligned} \frac{1}{N} \frac{d\phi^{TP}}{dz} = & (-65 \text{ rad} \cdot \text{fm}^2) [\bar{g}_\pi^{(0)} + 0.12 \bar{g}_\pi^{(1)} + 0.0072 \bar{g}_\eta^{(0)} \\ & + 0.0042 \bar{g}_\eta^{(1)} - 0.0084 \bar{g}_\rho^{(0)} + 0.0044 \bar{g}_\rho^{(1)} \\ & - 0.0099 \bar{g}_\omega^{(0)} + 0.00064 \bar{g}_\omega^{(1)}] \end{aligned} \quad (27)$$

and

$$\begin{aligned} P^{TP} = \frac{\Delta\sigma^{TP}}{2\sigma_{\text{tot}}} = & \frac{(-0.185 \text{ b})}{2\sigma_{\text{tot}}} [\bar{g}_\pi^{(0)} + 0.26 \bar{g}_\pi^{(1)} - 0.0012 \bar{g}_\eta^{(0)} \\ & + 0.0034 \bar{g}_\eta^{(1)} - 0.0071 \bar{g}_\rho^{(0)} + 0.0035 \bar{g}_\rho^{(1)} \\ & + 0.0019 \bar{g}_\omega^{(0)} - 0.00063 \bar{g}_\omega^{(1)}]. \end{aligned} \quad (28)$$

For a comparison, the DDH model of PV interaction with the AV18 + UIX strong potential at $E_{cm} = 100 \text{ keV}$ gives

$$\begin{aligned} \frac{1}{N} \frac{d\phi^P}{dz} = & (55 \text{ rad} \cdot \text{fm}^2) [h_\pi^1 + h_\rho^0(0.11) + h_\rho^1(-0.035) \\ & + h_\omega^0(0.14) + h_\omega^1(-0.12) + h_\rho^1(-0.013)] \end{aligned} \quad (29)$$

$$\begin{aligned} P^P = \frac{\Delta\sigma^P}{2\sigma_{\text{tot}}} = & \frac{(0.395 \text{ b})}{2\sigma_{\text{tot}}} [h_\pi^1 + h_\rho^0(0.021) + h_\rho^1(0.0027) \\ & + h_\omega^0(0.022) + h_\omega^1(-0.043) + h_\rho^1(-0.012)]. \end{aligned} \quad (30)$$

These expressions correspond to

$$\begin{aligned} \frac{1}{N} \frac{d\phi^P}{dz} = & (59 \text{ rad} \cdot \text{fm}^2) [h_\pi^1 + h_\rho^0(0.10) + h_\omega^0(0.14) \\ & + h_\rho^1(-0.042) + h_\omega^1(-0.12) + h_\rho^1(0.014)] \end{aligned} \quad (31)$$

TABLE II. The difference of scattering amplitudes $(f_+^{TP} - f_-^{TP})/(pC_n)$ for the TRIV potential operators $n = 1, 2, 4$, and 5 for mass scales corresponding to meson masses at $E_{cm} = 100$ keV. All numbers are in units of fm.

n	$\frac{\Delta f^\pi}{p}$	$\frac{\Delta f^\eta}{p}$	$\frac{\Delta f^\rho}{p}$	$\frac{\Delta f^\omega}{p}$
1	$-0.615 - i0.0567$	$-0.317 - i0.00738$	$-0.125 - i0.00329$	$-0.119 - i0.00317$
2	$-7.58 + i1.07$	$-0.761 + i0.0901$	$-0.302 + i0.0361$	$-0.288 + i0.0345$
4	$3.14 - i0.300$	$0.571 - i0.0227$	$0.225 - i0.00873$	$0.215 - i0.00832$
5	$-4.99 + i0.848$	$-0.262 + i0.0717$	$-0.0934 + i0.0273$	$-0.0888 + i0.0260$

in the zero-energy limit, and to

$$P^P = \frac{\Delta\sigma^P}{2\sigma_{\text{tot}}} = \frac{(0.140 \text{ b})}{2\sigma_{\text{tot}}} [h_\pi^1 + h_\rho^0(0.021) + h_\omega^0(0.022) + h_\rho^1(0.002) + h_\omega^1(-0.044) + h_\rho^1(-0.012)] \quad (32)$$

at $E_{cm} = 10$ keV, which were calculated using the DDH-II/AV18 + UIX potentials in Ref. [6]. The equations have the expected dependence of $\Delta\sigma^{TP}$ and $\Delta\sigma^P$ on neutron energy as $(E_n)^{1/2}$. The angle of the spin rotation, being proportional to the scattering length, is not sensitive to neutron energy in the low-energy regime.

The results of Table II could also be considered as an illustration of the cutoff dependence of matrix elements for the EFT calculations. However, physical observables do not depend on the cutoff due to the renormalization of $C_i^\pi = -\frac{c_i^\pi \mu^2}{2m_N}$. In the pionless EFT with cutoff $\mu = m_\pi$, the observables can be written in terms of dimensional LECs, c_i^π (in fm²), as

$$\begin{aligned} \frac{1}{N} \frac{d\phi^{TP}}{dz} &= (-2.45 \text{ rad}) [c_2^\pi + c_1^\pi(0.081) \\ &\quad + c_4^\pi(0.41) + c_5^\pi(0.66)], \\ P^{TP} &= \frac{\Delta\sigma^{TP}}{2\sigma_{\text{tot}}} = \frac{(-0.35)}{\sigma_{\text{tot}}} [c_2^\pi + c_1^\pi(-0.053) \\ &\quad + c_4^\pi(-0.28) + c_5^\pi(0.79)]. \end{aligned} \quad (33)$$

For the case of the pionful EFT, the one-pion-exchange contribution is considered explicitly, and all other cutoffs for contact terms should be larger than the pion mass. Therefore, the results in Table II for pion, ρ , and ω masses correspond to results for different μ 's. For example, by choosing the cutoff scale $\mu = m_\rho$, the expressions for TRIV observables are

$$\begin{aligned} \frac{1}{N} \frac{d\phi^{TP}}{dz} &= (-65 \text{ rad} \cdot \text{fm}^2) [\bar{g}_\pi^{(0)} + 0.12\bar{g}_\pi^{(1)}] \\ &\quad + (-3.05 \text{ rad}) [c_2^\pi + c_1^\pi(0.41) \\ &\quad + c_4^\pi(-0.75) + c_5^\pi(0.31)] \end{aligned} \quad (34)$$

and

$$\begin{aligned} P^{TP} &= \frac{\Delta\sigma^{TP}}{2\sigma_{\text{tot}}} = \frac{(-0.185 \text{ b})}{2\sigma_{\text{tot}}} [\bar{g}_\pi^{(0)} + 0.26\bar{g}_\pi^{(1)}] \\ &\quad + \frac{(-0.728)}{2\sigma_{\text{tot}}} [c_2^\pi + c_1^\pi(-0.091) \\ &\quad + c_4^\pi(-0.24) + c_5^\pi(0.76)]. \end{aligned} \quad (35)$$

It should be noted that all existing calculations of TRIV couplings are based on the meson-exchange model since EFT low-energy constants for TRIV interactions are unknown. By using the meson-exchange model, one can predict TRIV effects for different mechanisms of CP violation because the values of the TRIV meson-nucleon coupling constants depend on the model of CP violation.

The results of the calculations show that the dominant contributions to TRIV effects come from the first five operators. Moreover, in the meson-exchange formalism, the pion-exchange contribution is dominant, provided that CP -odd coupling constants for all mesons have the same order of magnitude. Thus, comparing Eqs. (27) and (28) with (29) and (30), one can see that contributions from ρ and ω mesons to TRIV effects are suppressed by about one order of magnitude in comparison to the contributions of these mesons to PV effects. This fact is especially interesting because, in the majority of models of CP violation, TRIV pion-nucleon coupling constants are much larger than ρ and ω ones (for details see, for example, [19–22] and references therein.) Assuming that the dominant contributions come from π mesons and using the conventional parameter [8,23] $\lambda = \bar{g}_\pi/h_\pi^1$, one can describe the TRIV observables in terms of the corresponding PV observables as

$$\begin{aligned} \frac{\phi^{TP}}{\phi^P} &\simeq (1.2) \left(\frac{\bar{g}_\pi^{(0)}}{h_\pi^1} + (0.12) \frac{\bar{g}_\pi^{(1)}}{h_\pi^1} \right), \\ \frac{\Delta\sigma^{TP}}{\Delta\sigma^P} &\simeq (-0.47) \left(\frac{\bar{g}_\pi^{(0)}}{h_\pi^1} + (0.26) \frac{\bar{g}_\pi^{(1)}}{h_\pi^1} \right). \end{aligned} \quad (36)$$

These ratios of TRIV and PV parameters do not depend on neutron energy.

It is useful to relate these estimates to the existing experimental constraints obtained from electric dipole moment measurements, even though the relationships are model dependent. For example, the CP -odd coupling constant $\bar{g}_\pi^{(0)}$ could be related to the value of the neutron electric dipole moment d_n generated via a π^- loop in the chiral limit [24] as

$$d_n = \frac{e}{4\pi m_N} \bar{g}_\pi^{(0)} g_\pi \ln \frac{\Lambda}{m_\pi}, \quad (37)$$

where $\Lambda \simeq m_\rho$. Then, using the experimental limit [25] on d_n , one can estimate $\bar{g}_\pi^{(0)}$ as less than 2.5×10^{-10} . The constant $\bar{g}_\pi^{(1)}$ can be bounded using the constraint [26] on the ^{199}Hg atomic EDM as $\bar{g}_\pi^{(1)} < 0.5 \times 10^{-11}$ [27].

Theoretical predictions for λ can vary from 10^{-2} to 10^{-10} for different models of CP violation. See, for example, [8,19–21,23] and references therein. Therefore, one can estimate a range of possible values of the TRIV observable and relate a particular mechanism of CP violation to their values. It should be noted that the above parametrization assumes that the π -meson-exchange contribution is dominant for PV effects. Should the $\vec{n} + p \rightarrow d + \gamma$ experiment confirm the “best value” of the DDH pion-nucleon coupling constant h_π^1 , Eqs. (36) can be considered as an estimate for the value of TRIV effects in neutron-deuteron scattering. Otherwise, if h_π^1

is small, one needs to use h_ρ or h_ω with corresponding weights, which will increase the relative values of TRIV effects.

ACKNOWLEDGMENTS

This work was supported by the DOE Grant No. DE-FG02-09ER41621. This work was granted access to the HPC resources of IDRIS under the allocation 2009-i2009056006 made by GENCI (Grand Equipement National de Calcul Intensif). We thank the staff members of the IDRIS for their constant help.

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