Microscopic T-Violating Optical Potential: Implications for Neutron-Transmission Experiments

J. Engel,1 C. R. Gould,2 and V. Hnizdo3

1Department of Physics and Astronomy, University of North Carolina, Chapel Hill, North Carolina 27599
2Department of Physics, North Carolina State University, Raleigh, North Carolina 27695
and Triangle Universities Nuclear Laboratory, Durham, North Carolina 27708
3Department of Physics and Schonland Research Centre for Nuclear Sciences, University of the Witwatersrand, Johannesburg, 2050 South Africa
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We derive a T-violating P-conserving optical potential for neutron-nucleus scattering, starting from a uniquely determined two-body ρ-exchange interaction with the same symmetry. We then obtain limits on the T-violating ρ-nucleon coupling \( \tilde{g}_\rho \) from neutron-transmission experiments in \(^{165}\text{Ho}\). The limits may soon compete with those from measurements of atomic electric-dipole moments.

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Several experimental groups have recently scattered polarized neutrons with low energies from heavy nuclei in search of parity or time-reversal violation [1]. The time-reversal experiments, requiring oriented targets, are the more difficult to perform. So far the only published measurements of this kind [2] have used neutron beams of several MeV and aligned \(^{166}\text{Ho}\) targets to search for a dependence of the forward elastic-scattering amplitude on the “fivefold” T-violating P-conserving (TVPC) correlation term \( \mathbf{s} \cdot (\mathbf{I} \times \mathbf{\hat{p}})(\mathbf{I} \cdot \mathbf{\hat{p}}) \). Here, \( \mathbf{I} \) and \( \mathbf{s} \) are unit vectors along the axes of the target alignment and neutron polarization, and \( \mathbf{\hat{p}} \) is the direction of the incident neutron beam. The correlation in the forward amplitude shows up as a change in the total cross section—related to the amplitude through the optical theorem—when the polarization of the incident neutron spin is reversed.

Until now there has been no credible way to connect these experiments to fundamental sources of \( T \) violation. Within the standard model TVPC effects must be tiny, but in extended models this may not be the case. Here we take an important first step in using neutron-transmission experiments to test any such models: Through the construction of a microscopic \( T \)-violating optical potential, we show how to relate the TVPC observable \( A_T \) [3] (connected to the difference between total cross sections for spin-up and spin-down neutrons on an aligned target) to TVPC meson-nucleon coupling constants. The problem of constraining fundamental models of \( T \) violation then reduces to physics at the meson or nucleon scale—namely a description of the effective TVPC vertex in terms of quarks and gluons.

In the case of parity violation, a number of mesons (\( \pi, \rho, \omega, \) etc.) contribute to the force between nucleons, which in turn determines the optical potential. Fortunately for us, the TVPC interaction is severely constrained. Simonius showed some time ago [4] that only the \( \rho \) and \( A_1 \) (or heavier) mesons can contribute at tree level; one-pion exchange, for example, is not allowed. Moreover, the form of the \( \rho \)-exchange potential is unique. The \( A_1 \)-exchange force is less constrained, but \( A_1 \) is significantly heavier than \( \rho \), and so its effects are damped by short-range nucleon-nucleon repulsion. We therefore restrict our attention to \( \rho \) exchange; the techniques we use can just as easily be applied to \( A_1 \).

The unique TVPC \( \rho \)-exchange interaction is [4,5]

\[
V_{\rho}^{12} = \sum_{\nu} \frac{m_\rho^2 g_{\rho}^2 s_\nu}{4\pi M^2} \frac{\sigma_1 \cdot \sigma_2}{r_{12}} (1 + m_\nu r_{12}) (\sigma_1 - \sigma_2) \cdot \mathbf{l},
\]

where \( r_{12} = r_1 - r_2 \), \( \mathbf{l} = r_{12} \times \tfrac{1}{2} (\mathbf{p}_1 - \mathbf{p}_2) \), \( \mu_\nu = 3.70 \mu_N \) (\( \mu_N \) is the nucleon magnetic moment) is the isovector nucleon magnetic moment, \( M \) is the nucleon mass, \( g_{\rho} = 2.79 \) is the normal strong \( pNN \) coupling, and \( \tilde{g}_\rho \) is a dimensionless ratio of the TVPC coupling to \( g_{\rho} \). This notation is taken from Ref. [5], where limits on \( \tilde{g}_\rho \) were deduced from limits on the electric dipole moments of the neutron and \(^{199}\text{Hg}\).

The potential in Eq. (1) has a number of peculiarities. The isospin piece \( \sum_{\nu} \) is solely responsible for the \( T \) violation through the factor \( r \), implies that neutrons interact only with protons and that the direct part of any two-nucleon matrix element vanishes. In addition, the space-spin part of the interaction, while Hermitian, is antisymmetric in the nucleon coordinates. Combined with the spin dependence of the force, these features have important consequences for the strength of the neutron-nucleus TVPC optical potential \( \tilde{\mathcal{U}}(r) \), which we now proceed to evaluate.

We begin by considering a closely related quantity \( \tilde{\mathcal{M}}(r) \), the ground-state expectation value of the interaction \( V_{\rho}^{12} \):

\[
\langle \psi_a | \tilde{\mathcal{M}} | \psi_b \rangle = \langle \psi_a | \Psi_A \rangle \sum_{\rho} V_{\rho}^{12} | \psi_b | \Psi_A \rangle.
\]

where the index \( \rho \) refers to the incident neutron, \( | \psi_a \rangle \) and \( | \psi_b \rangle \) are arbitrary neutrons states, the index \( \rho = 2, 3, \ldots, Z + 1 \) labels protons in the nucleus, \( | \Psi \rangle \) is the nuclear ground state, and the subscript \( A \) means that the matrix element is completely antisymmetrized. The
optical potential itself, $\hat{U}(r)$—in the so-called “adiabatic approximation” [6]—is a function of the nuclear-spin operator $\mathbf{I}$, the neutron-spin operator $\mathbf{s} = \frac{1}{2} \vec{\sigma}$, and the neutron position $r$, defined so that the ground-state nuclear matrix element of $\hat{U}$ is $\hat{M}$. This definition, which amounts to treating the nucleus as an elementary particle with spin $J$, is necessary for making contact with the usual phenomenology, where terms that depend on the nuclear spin (e.g., $\vec{\sigma} \cdot \mathbf{I}$) appear in the optical potential.

A number of authors have derived similar one-body potentials—usually felt by bound nucleons [7]—in the approximation just described. Unfortunately, the unusual features of $V^p$ make the same kind of calculations more complicated here. If the nuclear wave function is approximated as usual by a Slater determinant, then

$$\langle r_1 | \hat{M} | r_2 \rangle = 2i \sum_p \langle r_1 | (\phi_p) \Gamma_{12}^p | \phi_p \rangle \langle r_2 | ,$$

(3)

where the $| \phi_p \rangle$ are occupied proton orbits. Equation (3) sums only exchange matrix elements in coordinate and

$$\langle \psi_a | \hat{M} | \psi_b \rangle \sim \frac{G_{\pi}^a G_{\rho}^{\mu \nu}}{m_p^2 M^2} \sum_{p, k} \int d^3r \phi_a^\dagger(r) \left[ [\vec{\sigma} \cdot \nabla \phi_p(r) \times \nabla \phi_a^\dagger(r)] - \nabla \times [\phi_p(r) \phi_a^\dagger(r)] \cdot \nabla \right] \psi_b(r) ,$$

(5)

where the derivatives act only on the functions immediately next to them, and the square brackets indicate commutators, combined in the first term with a dot product. $\hat{M}(r)$ is now just the operator in parentheses above. Noting that the $\phi_p(r)$ are two-component spinors ($\phi^{\dagger}$ is an outer product), we use trace identities to obtain

$$\hat{M}(r) = \frac{2G_{\pi}^a G_{\rho}^{\mu \nu}}{m_p^2 M^2} \sum_{p, k} \mathbf{R} [i \nabla \phi_p^\dagger(r) \vec{\sigma} \cdot \nabla \phi_p(r)] \sigma_k ,$$

(6)

where $k$ labels Cartesian components. We have dropped two other terms, coming from the second term in Eq. (5), which change sign when the nuclear spin is reversed. Since the fivefold correlation itself is invariant under reversal of the nuclear spin direction, the neglected terms can contribute only in conjunction with a potential like $\vec{\sigma} \cdot \mathbf{I}$, which rectifies their spin-reversal behavior. Such terms do exist in the normal optical potential [9], but are substantially weaker than the central potential. If we imagine treating them together with our TVPC potential as perturbative corrections in the distorted-wave Born approximation, it is clear that the term we have kept in Eq. (6), which already has

$$Z_{n, l, j, j'}(r) = \sqrt{2l' + 1} \pm 2 \begin{pmatrix} \frac{2}{1/2} & \frac{l' + 1}{j} \\ \frac{1}{2} & \frac{l}{j} \end{pmatrix} \left[ \sqrt{(l + 1)(2l + 1)} \begin{pmatrix} \frac{2}{l + 1} & \frac{l' + 1}{2} \\ \frac{l}{2} & \frac{l'}{1} \end{pmatrix} \right] \begin{pmatrix} \frac{2}{l} & \frac{l' - 1}{0} \\ \frac{1}{l} & \frac{l'}{0} \end{pmatrix} R_{n, l, j}(r)$$

$$- \sqrt{(2l - 1)} \begin{pmatrix} \frac{2}{l - 1} & \frac{l' - 1}{2} \\ \frac{l - 1}{2} & \frac{l'}{1} \end{pmatrix} \begin{pmatrix} \frac{2}{l - 1} & \frac{l' + 1}{0} \\ \frac{l}{l - 1} & \frac{l'}{0} \end{pmatrix} R_{n, l, j}(r) \right] R_{n', l', j'}(r) ,$$

(8)

the right symmetry, will dominate those we have omitted.

Some of the potential’s unusual properties follow directly from Eq. (6). If, for example, the $\phi_p(r)$ come from a spherical potential, then $\hat{M}$ and $\hat{U}$ vanish in a spin-saturated or closed-$J$-shell nucleus. Thus, only a few valence protons in the last orbital contribute to $\hat{U}$. A spherical mean-field treatment, in fact, makes sense only in closed-shell or closed-shell-plus-one nuclei, so that in this simple picture at most one nucleon, characterized, e.g., by a valence orbital with quantum numbers $n, l, j$, is relevant. Using standard angular-momentum algebra, properties of spherical harmonics, etc., one can write down an explicit expression for the $\hat{M}$ generated by the valence orbital and then for the corresponding optical potential $\hat{U}$. For $j = l \pm 1/2$ we have

$$\hat{U}(r) = \frac{5 \pi^{-1} \sqrt{30} j(1-j)^{-1/2} G_{\pi}^a G_{\rho}^{\mu \nu}}{\sqrt{j(j + 1)(2j - 1)(2j + 3)m_p^2 M^2} Z_{n, l, j}(r) T_j} ,$$

(7)

where $a = \sqrt{2a + 1}$ and $Z_{n, l, j}(r)$ is the diagonal component of a matrix we will use again below ($j' = l' \pm 1/2$).
The $R_{nlj}^\pm$ are related to the radial wave functions $R_{nlj}$ by
\[
R_{nlj}^\pm(r) = \left( \frac{3}{\partial r} \mp \frac{l + 1/2}{r} \mp 1/2 \right) R_{nlj}(r). \tag{9}
\]
The factor $T_5$ in Eq. (7) is the fivefold operator
\[
T_5 = \frac{1}{2} r^{-2} \{ s \cdot (\mathbf{I} \times r)(\mathbf{I} \cdot r) + (\mathbf{I} \cdot r)(\mathbf{I} \times r) \cdot s \}
\]
\[
- i \sqrt{\pi} \left[ (\mathbf{I} \times \mathbf{r})^2 \times (\mathbf{z} \times \mathbf{r})^2 \right]^{1/2}, \tag{10}
\]
where the square brackets now mean that the angular momenta are coupled. [We have omitted from Eq. (7) other terms that have no effect when the target is only rank-2 aligned.] The presence of $T_5$ in Eq. (7) is interesting; it was proposed without microscopic justification in Ref. [3] solely because of its TVPC tensorial structure. The radial form of Eq. (7), however, is quite different from the

\[
\hat{U}(r) = \frac{10 \pi^{-1} \sqrt{30} (-1)^{l+k} g^{-2} g_{\rho}^{2} \mu_{u}}{\sqrt{I(I+1)(2I-1)(2l+1)I_0^3}} \begin{pmatrix} I & I & 2 \\ -K & K & 0 \end{pmatrix}
\]
\[
\times \left[ \sum_{\alpha \beta} \alpha \beta (\mathbf{I} \times \mathbf{r})^{2} \times (\mathbf{z} \times \mathbf{r})^{2} \right]^{1/2} T_5, \tag{11}
\]

where $I = 7/2$ is the nuclear spin, $K = 7/2$ is the $z$ projection in the intrinsic frame, and the $a$'s are spherical expansion coefficients for the deformed single-particle orbital labeled by $\Omega$. Even though all such orbits in the valence shell now contribute to $\hat{U}$, in the end the strength of the potential is still comparable to that arising from a single spherical orbital. Figure 1 shows the potential's radial shape. The curve looks very different from a typical volume or surface optical potential, reflecting the nonlocality discussed above. It is small at both the origin and the surface, peaking somehow in between.

Including the TVPC potential alongside the strong optical potential $U$ [3] in, e.g., the coupled-channels code CHUCK [11], we can calculate the spin-correlation coefficient $A_5$ for any value of $g_{\rho}$, or vice versa. Figure 2 shows $A_5$ as a function of neutron energy for $g_{\rho} = 1$. The published measurement of $A_5$ at 2 MeV [2] results in an upper limit on $g_{\rho}$ of about 0.5, a value that must be increased by a factor of about 3 to account for short-range repulsion [5], which we have so far neglected. The additional analysis in Ref. [5] then implies a limit on $a_T$, the ratio of typical $T$ violating to strong two-body matrix elements, of about $1.5 \times 10^{-2}$. A recently completed experiment has improved the bound on $A_5$ by a factor of about 15, however [12], and a further order of magnitude is anticipated, potentially resulting in bounds on $a_T$ of order $10^{-4}$; this would make neutron-transmission experiments competitive with measurements of atomic dipole moments. Reference [5] also derives another limit, roughly an order of magnitude smaller still,
from measurements of the neutron dipole moment, but that value depends on the parity-violating pion-nucleon coupling, the size of which has been estimated [13] but is not known reliably.

In Ref. [3], a Woods-Saxon shape was used for the radial potential multiplying $T_3$ under the assumption that the potential is proportional to the nuclear density. A limit was then obtained on $\alpha_T$ by dividing the strength of the phenomenological TVPC potential (determined by calculating $\Delta_3$ in the same way as is done here) by that of the central optical potential. Our results show that this procedure yields too small a limit by about 2 orders of magnitude. Our TVPC potential is generated in lowest order by at most a few nucleons in the valence shell—hence the different shape and considerably larger upper limit on $\alpha_T$. A more appropriate way to extract a rough limit from a phenomenological potential would be to divide its strength not by the strength of the central potential, but instead by the strength of a symmetry-conserving spin-spin term such as $[(I \times I) \times (I \times I)]^2$, which resembles our TVPC interaction. In general, spin-spin interactions are $\approx 100$ times weaker than central interactions because they too are generated only by valence nucleons.

How reliable are the present results? The adiabatic approximation of Eq. (2) ignores higher-order (in $V_{\text{strong}}$) processes in which intermediate nuclear or neutron states are virtually excited and deexcited. Although such terms would alter our potential, we do not expect extremely large changes. Any coherent (higher-order) one-body potentials must be independent of the nuclear spin $I$ and therefore can affect $I$-dependent correlations only when acting together in perturbation theory with some other $I$-dependent force. Higher-order contributions to $\bar{U}$ that are themselves $I$ dependent should be suppressed by amounts typical of Bruckner-Bethe-Goldstone perturbation theory. Additionally, working in a deformed basis takes into account at least some of the important nuclear correlations. Our potential is therefore probably correct to within factors of order unity.

Several times we have noted that $T$-odd potentials generated by the core will not contribute by themselves to $T$-dependent observables in lowest order. This statement, which is true whether the potentials are $P$ even or $P$ odd, does not, however, appear to be relevant for epithermal neutrons because in a compound nucleus $I$-dependent terms can no longer be treated as perturbative corrections. On the other hand, because of the complicated structure of compound-nucleus resonances, there is no simple connection of the kind established here between experimental observables and $T$-odd forces. It therefore remains to be seen whether experiments with epithermal neutrons can constrain TVPC couplings as reliably as experiments at higher energies.

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