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Nuclear spin-independent effects of parity nonconservation in molecule of hydrogen

D V Chubukov^{1,2} , L V Skripnikov^{1,2}, L N Labzowsky^{1,2} and G Plunien³

¹Department of Physics, St. Petersburg State University, 7/9 Universitetskaya Naberezhnaya, Saint Petersburg 199034, Russia

²Petersburg Nuclear Physics Institute named by B.P. Konstantinov of National Research Centre 'Kurchatov Institut', St. Petersburg, Gatchina 188300, Russia

³Institut für Theoretische Physik, Technische Universität Dresden, Mommsenstrasse 13, D-01062, Dresden, Germany

E-mail: dmitrybeat@gmail.com

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Abstract

Theoretical concepts and calculation results of the spatial parity nonconserving (PNC) effects of electron-electron and electron-nucleus nuclear spin-independent interactions in diatomic homonuclear molecule H₂ of parahydrogen are presented. The magnetic dipole transition between the states with the same rotational number of the vibrational $\nu = 1 \leftarrow 0$ band in the H₂ ground electronic $^1\Sigma_g^+$ state is considered. It is shown that in this situation these effects are of the same order of magnitude. The H₂ molecule is therefore the first example of molecular system where the electron-electron PNC interaction can be directly observed. Since the constants of the electron-nucleus PNC interaction have been already accurately measured in atomic experiments, the electron-electron PNC interaction constant also can be extracted from the future experiments. In other atoms and molecules the electron-electron PNC interaction is usually deeply screened by the electron-nucleus one. Since the nuclei of H₂ contain no neutrons, in such future experiments on the PNC effect observation one can, in principle, measure the Weinberg angle (free parameter of the standard model) with unprecedented accuracy.

Keywords: parity nonconservation, hydrogen molecule, electron-electron weak interaction

1. Introduction

A theoretical study of the discrete symmetry (e.g. spatial parity \mathcal{P}) violation effects in atomic and molecular systems plays a key role in developing theories and models of fundamental interaction physics. The standard model (SM) of electroweak interactions was established in the 1960s [1–3] after the neutral weak current hypothesis had been proposed. The claim of the SM stimulated to look for and measure weak interaction effects in atomic and molecular systems. It should be stressed that in order to extract the values of the SM constants (namely the Weinberg angle) from the atomic experimental data, it is required to perform accurate theoretical calculations. These calculations are considerably sophisticated since all electrons can contribute. As a matter of fact, experiments on the search for parity nonconservation (PNC) in atomic and molecular systems can be divided into two research directions: observation of the optical dichroism

(i.e. asymmetry of the number of emitted or absorbed right and left circularly polarized photons) and optical rotation of the light polarization plane in vapor of atoms and molecules which do not possess natural optical activity. The experiment along the first research direction was suggested by M Bouchiat and C Bouchiat on neutral cesium atom in 1974 [4] and carried out by the Wieman group in 1997 [5]. To date it is the most accurate low-energy experiment that validates the correctness of the SM. The experiment of the second type was proposed by Khriplovich on the bismuth atom in 1974 [6]. For a comprehensive list of the relevant PNC experiments see, for example, the review [7]. Due to the difficulties of theoretical calculations of \mathcal{P} -odd effects in heavy atoms the search for simpler atomic systems where effects of the same size occur are of interest. It is well-known that PNC electron-nucleus (e -N) interaction effect in neutral atoms increases with the nuclear charge Z approximately as Z^3 [4, 8]. That is why, the most appropriate choice can be few-electron heavy

highly charged ions (HCI) which combine the advantage of high Z numbers with the absence of correlation problem. The first proposal to measure \mathcal{P} -odd effects in He-like HCI was made in [9] and was stimulated by the crossing of levels with opposite parity at $Z \sim 6, 30, 64, 90$. Series of papers on searching for the PNC effects in HCI was published during the last few decades. Unfortunately, no experiments with HCI have been carried out up to now. Here we only want to note that recently in [10] a new PNC experiment with HCI in storage rings has been suggested. The main advantage of the experiment is the employment of the new method for polarizing the HCI nuclei, namely by the capture of polarized electrons.

In all these atomic experiments only the \mathcal{P} -odd e -N interaction was observed or proposed since it is enhanced in heavy atoms, while the \mathcal{P} -odd electron-electron (e - e) interaction is negligible in these cases [4, 8, 11, 12]. The \mathcal{P} -odd interaction of electrons with each other was observed exclusively in the high energy region in elastic Møller scattering of a polarized electron beam on an unpolarized electron target in 2005 by the SLAC-E158 collaboration [13]. No other evidence for the existing of the parity violating e - e weak interaction has ever been reported and the independent observation of this effect in the low-energy regime to our mind would be desirable.

In 1977 it was suggested to observe the effect of the \mathcal{P} -odd optical rotation on the O_2 molecule [14]. According to rough estimates it was claimed that this effect arises mainly due to the weak e - e interaction. The idea was as follows: in a molecule there should be a strong enhancement of the effect because all electrons involving in the formation of a chemical bond are inside the internuclear region. Recently, calculation of the \mathcal{P} -odd effects in O_2 has been performed in [15]. It appears that the \mathcal{P} -odd e -N interaction effect prevails over the \mathcal{P} -odd e - e interaction one by 2 orders of magnitude for this case. The \mathcal{P} -odd interactions are short-ranged. Therefore, due to the weak overlap between electron wave functions with different orbital angular momenta (states with opposite spatial parities that are mixed via weak interactions) and the Z^3 dependence of the PNC e -N interaction effect [4, 8], in neutral atoms the PNC e - e interaction can be even more suppressed compared to the PNC e -N one than in this case of the oxygen molecule. Therefore, the idea about the possible enhancement of the \mathcal{P} -odd e - e interaction in diatomic homonuclear molecules is valid by itself. Taking into account all above-mentioned, lighter diatomic molecules should be investigated for the search of the e - e PNC effect.

The aim of this paper is to perform *ab initio* calculations of the nuclear spin-independent PNC effects in parahydrogen H_2 , in which the spins of protons are antiparallel, so the total nuclear spin is zero. It is obvious that in the parahydrogen the nuclear spin-dependent PNC interaction effects vanish. We consider the magnetic dipole (M1) transition between the states of the same rotational quantum number N of the vibrational $v = 1 \leftarrow 0$ band in the H_2 ground electronic $X^1\Sigma_g^+$ state (X stands for the spectroscopic notation of the ground state). Ungerade u and gerade g parities under

inversion of electron coordinates alone while the coordinates of nuclei held fixed exist only in homonuclear molecules. Until recently these transitions were assumed to be only of the electric quadrupole (E2) type so in such situation PNC experiments would be meaningless. The admixture of the PNC-induced electric dipole (E1) transition amplitude to magnetic dipole amplitude via weak interactions is favourable for the PNC effect observation. Recently in [16] it has been shown that magnetic dipole transitions also take place for such transitions, although they are significantly weaker than the ordinary atomic ones.

2. Theory

In this section we consider the mechanism of the spatial parity violation as applied to the case of the M1 transition between $v_1 = 1$ and $v_0 = 0$ vibrational levels with the same rotational number $N = J$ (\mathbf{N} is the total angular momentum (including the rotational one) excluding the electron spin, \mathbf{J} is the total angular momentum of a molecule) of the ground electronic $^1\Sigma_g^+$ state of the H_2 molecule.

Due to the \mathcal{P} -symmetry violation induced by an effective operator of PNC interaction $V_{\mathcal{P}}$ the gerade wave function of the H_2 ground state $\psi_{g v_0(v_1)J}$ ($|g v_0(v_1)J\rangle$) gets the following admixture

$$\psi_{g v_0(v_1)J} \rightarrow \psi_{g v_0(v_1)J} + \sum_{i,j,k} \frac{\langle u_i v_j N_k J | V_{\mathcal{P}} | g v_0(v_1) J \rangle}{E_{g v_0(v_1)J} - E_{u_i v_j N_k J}} \psi_{u_i v_j N_k J}, \quad (1)$$

where $\psi_{u_i v_j N_k J}$ ($|u_i v_j N_k J\rangle$) are the i th ungerade wave functions (with parity opposite to the ground state one), $E_{u_i v_j N_k J}$ and $E_{g v_0(v_1)J}$ are the corresponding rovibronic energies. The PNC-induced mixing of the states leads to appearance of the pseudoscalar term in the probability of the process considered. The only pseudoscalar term that can be constructed is $(s_{ph} \cdot \nu)$, where $s_{ph} = i(\mathbf{e} \times \mathbf{e}^*)$ is the photon spin, ν is the photon emission direction, \mathbf{e} is the photon polarization. Then the probability can be expressed as

$$W = W^{M1}(1 + (s_{ph} \cdot \nu)\mathcal{P}). \quad (2)$$

Here \mathcal{P} is referred to as the degree of parity nonconservation, or the degree of circular polarization. In general

$$i\mathcal{P} = 2 \frac{E1_{g v_1 \rightarrow g v_0}^{PNC}}{M1_{g v_1 \rightarrow g v_0}}, \quad (3)$$

where $E1_{g v_1 \rightarrow g v_0}^{PNC}$, $M1_{g v_1 \rightarrow g v_0}$ are the PNC-induced amplitudes of an electric dipole transition and the amplitude of a magnetic dipole transition between the states of the same parity (g), respectively. In equation (3) the pseudoscalar term is supposed to be extracted. In fact, $E1 \sim \mathbf{d} \cdot \mathbf{e}$ and $M1 \sim \boldsymbol{\mu} \cdot (\mathbf{e} \times \nu)$. Here \mathbf{d} and $\boldsymbol{\mu}$ are the electric dipole and the magnetic dipole operators, respectively. Expanding the scalar products in spherical components and performing the angular reduction it can be shown that the factor $(s_{ph} \cdot \nu)$ can be

easily extracted. Then $E_{f,gv_1 \rightarrow gv_0}^{\text{PNC}}$ reads

$$E_{f,gv_1 \rightarrow gv_0}^{\text{PNC}} = \sum_{i,j,k} \left(\frac{\langle gv_1 J | (\mathbf{d})_f | u_i v_j N_k J \rangle \langle u_i v_j N_k J | V_{\mathcal{P}} | gv_0 J \rangle}{E_{gv_0 J} - E_{u_i v_j N_k}} + \frac{\langle gv_1 J | V_{\mathcal{P}} | u_i v_j N_k J \rangle \langle u_i v_j N_k J | (\mathbf{d})_f | gv_0 J \rangle}{E_{gv_1 J} - E_{u_i v_j N_k}} \right). \quad (4)$$

By the letter f a spherical component of \mathbf{d} is denoted. Because of the \mathcal{T} -invariance of the interaction, the \mathcal{P} -odd matrix element is purely imaginary [8]. Due to different multiplicity, E2 doesn't interfere neither with M1 nor with E1 transition amplitudes, therefore as it was shown in [8] the rotation angle φ of the light polarization plane does not depend on the presence of E2 amplitude, only the light absorption length does.

In the coordinate space within the SM, the \mathcal{P} -odd effective e - e interaction and the \mathcal{P} -odd effective nuclear spin-independent e -N interaction operators can be expressed in the following forms, respectively:

$$V_{ee} = \frac{G_{ee}}{\sqrt{2}} (\gamma_{\mu})_1 (\gamma_{\mu})_2 \delta(\mathbf{r}_1 - \mathbf{r}_2) + (1 \rightleftharpoons 2) \\ = \frac{G_{ee}}{\sqrt{2}} ((\gamma_5)_1 + (\gamma_5)_2 - \alpha_1 \Sigma_2 - \alpha_2 \Sigma_1) \delta(\mathbf{r}_1 - \mathbf{r}_2), \\ V_{eN} = -\frac{G_{eN}}{2\sqrt{2}} \gamma_5 (\rho(\mathbf{r}) + \rho(\mathbf{r} - \mathbf{R})). \quad (5)$$

Here $G_F = 1.027 \cdot 10^{-5} \hbar c \left(\frac{\hbar}{m_p c} \right)^2 = 2.222 49 \cdot 10^{-14}$ a.u. is the Fermi constant (where m_p is the proton mass), the e - e weak interaction constant $G_{ee} = G_F \cdot (1 - 4 \sin^2 \theta_W)$ (where θ_W is the Weinberg angle—free parameter of the SM), the e -N weak interaction constant $G_{eN} = G_F Q_W$, R is the internuclear distance. For the purposes of our work, the Weinberg angle can be approximated as $\sin^2 \theta_W \approx 0.23$. Thus, $G_e \approx 0.08 G_F$. γ_{μ} , γ_5 , α , Σ are the Dirac matrices, Q_W is the weak charge of nucleus

$$Q_W = -N + Z(1 - 4 \sin^2 \theta_W), \quad (6)$$

N , Z are the numbers of neutrons and protons in a nucleus, respectively; $\rho(\mathbf{r})$ is the normalized nuclear density distribution.

The hydrogen molecule conforms very closely to Hund's coupling scheme (b) which corresponds to the weak spin-orbit coupling interaction compared to the difference between rotational sublevels (or rotational constant). For the case (b) the projection of the orbital electronic angular momentum on the internuclear axis, Λ , is a good quantum number while the projection of the total electronic angular momentum on the internuclear axis, Ω , is not. The \mathcal{P} -odd effective operators given by equation (5) are electronic scalars, therefore the matrices of these operators are diagonal in Ω . It means that these operators can be conveniently considered in the space of Hund's case (a) basis functions. Coupling scheme (a) corresponds to the strong spin-orbit coupling interaction compared to the difference between rotational sublevels. But it should

be noted that these schemes play a role of the basis sets. For our purposes it is convenient to make a transformation from (b) basis set to (a) one (see, e.g. [17]) and perform further calculations in Hund's coupling scheme (a).

The ground $^1\Sigma_g^+(0_g^+)$ state of parahydrogen (with the standard notation in brackets $\Omega_{g(u)}^{\pm}$) possesses only even rotational quantum numbers $N = J$ [18]. The electronic configuration of H_2 ground state $\psi(^1\Sigma_g^+)$ is $(1\sigma_g)^2$. The \mathcal{P} -odd nuclear spin-independent operators in equation (5) cannot mix ortho- and para-states. For a given $^1\Sigma_g^+(0_g^+)$ ground state these interactions lead to the admixture of such $^{2S+1}\Lambda_u^{\pm}$ states in terms of (b) basis functions, which have nonzero projection on the 0_u^- states in the (a) basis set.

It is known that in H_2 all Σ states have Σ^+ symmetry [18]. However, the $^3\Sigma_u^+$ para-state (with odd N quantum numbers) includes the 0_u^- state in terms of Ω due to spin multiplicity and thus also can be admixed to the ground para-state via the \mathcal{P} -odd effective operators given in equation (5). Due to the parity, in fact, Π states become a linear combination of $\Lambda = 1$ and $\Lambda = -1$ states. As the result, only $^3\Pi_u^- = \frac{1}{\sqrt{2}}(|\Lambda = 1\rangle - |\Lambda = -1\rangle)$ (with even N) and $^3\Sigma_u^+$ (with odd N) para-states can contribute to the PNC effects.

The \mathcal{P} -odd interaction results in the interference between M1 and PNC-induced E1 transition amplitudes. The next step is to derive an explicit expression for them in the considered transition. Applying the Wigner-Eckart theorem, the M1 transition amplitude reads

$$M1_{q,gv_1 \rightarrow gv_0} = \langle JM'_J v_1 (^1\Sigma_g^+) | (\mu)_q | JM_J v_0 (^1\Sigma_g^+) \rangle \\ = (-1)^{J-M'_J} \cdot \begin{pmatrix} J & 1 & J \\ -M'_J & q & M_J \end{pmatrix} \cdot \langle gJv_1 || \mu || gJv_0 \rangle. \quad (7)$$

Here $\langle gJv_1 || \mu || gJv_0 \rangle = \sqrt{J(J+1)(2J+1)} \mu_N \langle v_1 | g(R) | v_0 \rangle$ where μ_N is the nuclear magneton and g is the rotational g -factor. In fact, different vibrational functions corresponding to the same electronic state are orthogonal ($\langle v_1 | v_0 \rangle = 0$). It was shown in [16], however, that in the leading order of the nonadiabatic perturbation theory the g -factor depends on the internuclear distance R , hence such matrix elements are not zero. In this paper we used M1 amplitudes $\langle v_1 | g(R) | v_0 \rangle$ for different J from [16]. It appears that $\mu_N \langle v_1 | g(R) | v_0 \rangle \approx (4 - 5) \cdot 10^{-8} e a_0$ (e is the electron charge and a_0 is the Bohr radius) for $J = (2 - 30)$ that is, they depend only slightly on J .

In appendix the separation of the rotational part in the interference contribution of M1 and $E1^{\text{PNC}}$ transition amplitudes applied to the case of intermediate admixed $^3\Pi_u^-$ states is performed. It follows that

$$E_{gv_1 \rightarrow gv_0}^{\text{PNC}} = \frac{1}{2} \sqrt{\frac{2J+1}{2J(J+1)}} \\ \times \sum_{i,j} \left(\frac{\langle gv_1 | d(R) | u_i v_j \rangle \langle u_i v_j | V_{\mathcal{P}}(R) | gv_0 \rangle}{E_{gv_0} - E_{u_i v_j}} - \frac{\langle gv_1 | V_{\mathcal{P}}(R) | u_i v_j \rangle \langle u_i v_j | d(R) | gv_0 \rangle}{E_{gv_1} - E_{u_i v_j}} \right), \quad (8)$$

where

$$\begin{aligned} d(R) &= \langle g(0_g^+) | (\mathbf{d})_{-1} | {}^3\Pi_u(1_u) \rangle \\ &\quad - \langle g(0_g^+) | (\mathbf{d})_{+1} | {}^3\Pi_u((-1)_u) \rangle, \\ V_{\mathcal{P}}(R) &= \langle {}^3\Pi_u(0_u^-) | V_{\mathcal{P}} | g(0_g^+) \rangle. \end{aligned} \quad (9)$$

The operator $V_{\mathcal{P}}$ denotes both V_{ee} and V_{eN} operators. The similar derivations as in [appendix](#) can be performed for the case of mixing between intermediate ${}^3\Sigma_u^+$ (with odd N_k) and the ground state (with even rotational numbers). In this case $N_k = J \pm 1$. It can be shown that the contributions with $N_k = J - 1$ and $N_k = J + 1$ are equal in value but opposite in sign. More specifically, the only difference between these two contributions is negligibly small difference in energy denominators ($E_{v_1(v_0)J({}^1\Sigma_g^+)} - E_{v_j, N_k=J-1, ({}^3\Sigma_u^+)}$) and ($E_{v_1(v_0)J({}^1\Sigma_g^+)} - E_{v_j, N_k=J+1, ({}^3\Sigma_u^+)}$). Hence, only $n^3\Pi_u^-$ states noticeably can contribute to the NSI-PNC (nuclear spin-independent PNC) effects.

It should be also pointed out that according to equation (4) one should consider the singlet-triplet E1 amplitudes. Although such transitions are forbidden in the nonrelativistic approximation due to the spin selection rule $\Delta S = 0$, still since we take into account all relativistic effects in the framework of the Dirac–Coulomb Hamiltonian, the E1 amplitudes are not set to zero but are nevertheless quite small.

3. Electronic structure calculation details

Electronic structure calculations of the \mathcal{P} -odd matrix elements are performed here. For this aim the full configuration interaction method (FCI) and Dirac–Coulomb Hamiltonian were used to take complete account of electron correlation and relativistic effects for H_2 . The Breit interaction can be neglected in our case (e.g. in [19] it was shown that Breit correction in Cs atom for PNC amplitude is found to be 0.4%). For the H atoms in the H_2 molecule the dyall.aae4z basis set [20, 21] in case of the one-electron e -N PNC-effect and aug-cc-pvDZ basis set [22] in case of the two-electron e - e PNC-effect were employed to ensure the flexibility of the wave function description. The CI calculations were performed using the DIRAC12 [23] and MRCC [24, 25] codes. The molecular orbitals in the Hartree–Fock method were obtained using the DIRAC12 code with the Dirac–Coulomb Hamiltonian. The computation of the transition reduced density matrices of the first order (RDM-1) for the calculation of the \mathcal{P} -odd e -N operator matrix elements and of the second order (RDM-2) for the calculation of the \mathcal{P} -odd e - e ones and also the electric dipole moment matrix elements in the molecule-fixed frame were obtained using the MRCC code and the code developed in the present paper. The transition RDMs-2 were computed in the approach of 100% contribution of the reference determinant to the ground (initial) state wave function (actual contribution of 99.1% is close to it). Taking the trace product of the transition RDM with the matrix form of the \mathcal{P} -odd effective operator in equation (5) one obtains the \mathcal{P} -odd matrix elements $V_{\mathcal{P}}(R)$. In order to faithfully reproduce

Table 1. Comparison of the present paper results for the $X^1\Sigma_g^+$ and $c^3\Pi_u$ internuclear equilibrium distances, spectroscopic constants B_e and D_e , and also the electronic energy of the excited $c^3\Pi_u$ state with the experimental data [26].

	Present paper $X^1\Sigma_g^+$	Experimental data [26] $X^1\Sigma_g^+$	Present paper $c^3\Pi_u$	Experimental data [26] $c^3\Pi_u$
R (a_0)	1.407	1.401	1.954	1.96
T_e (cm^{-1})	–	–	97287	95838
B_e (cm^{-1})	58.4	60.853	30.7	31.07
D_e (cm^{-1})	0.043	0.047 1	0.018 2	0.019

the potential energy curve all matrix elements were obtained at 20 points of the internuclear distance.

It should also be noted that the MRCC code operates in the Hund’s coupling scheme (a) basis set in which Ω is a good quantum number. That is why all over performing the calculation of the E1^{PNC} it is convenient to make a transformation from (b) to (a) basis functions. The uncertainty of the electronic structure calculations presented here can be estimated as about 10% for the PNC e -N effect and as about 15% for the PNC e - e effect which is sufficient to the present purpose. For example, calculated internuclear equilibrium distances, spectroscopic constants for each state, electronic energy of the excited state agree within (5–10)% with previous studies and experimental data (see table 1).

4. Results and discussion

Let us turn to the results of the calculation. Only the contribution of the first $c^3\Pi_u^-$ ($1^3\Pi_u^-$) state was taken into account. Next highly excited states ($n^3\Pi_u^-$ with $n > 2$) are described by more diffuse functions in the basis set (i.e. extended Gaussian basis functions with a small exponent). Since also according to equation (4) the energy denominators for these states are larger, the total contribution of them to the PNC effects can be neglected in the framework of the uncertainty claimed. For obtaining the contribution of the intermediate $c^3\Pi_u^-$ state and reproducing potential energy curves at different internuclear distances R the electronic structure calculations were performed for $d(R)$, $V_{ee}(R)$, $V_{eN}(R)$ (20 points of curve). The dependencies of the imaginary component of the \mathcal{P} -odd e -N and e - e matrix elements, the dipole moment matrix element on the internuclear distance R (see equation (9)) are given in figures 1(a)–(b). For performing the averaging of $d(R)$, $V_{ee}(R)$ and $V_{eN}(R)$ over the vibrational wavefunctions of the ground and excited states the VIBROT code of MOLCAS was used [27]. In our calculations the total Franck–Condon factors for the first 20 discrete vibrational levels $\sum_{i=0}^{19} (\langle v=0(X^1\Sigma_g^+) | v_i(c^3\Pi_u) \rangle)^2 = 0.996$ and $\sum_{i=0}^{19} (\langle v=1(X^1\Sigma_g^+) | v_i(c^3\Pi_u) \rangle)^2 = 0.969$. Since these values are very close to unity, one can neglect the contribution of the continuum vibrational spectrum.

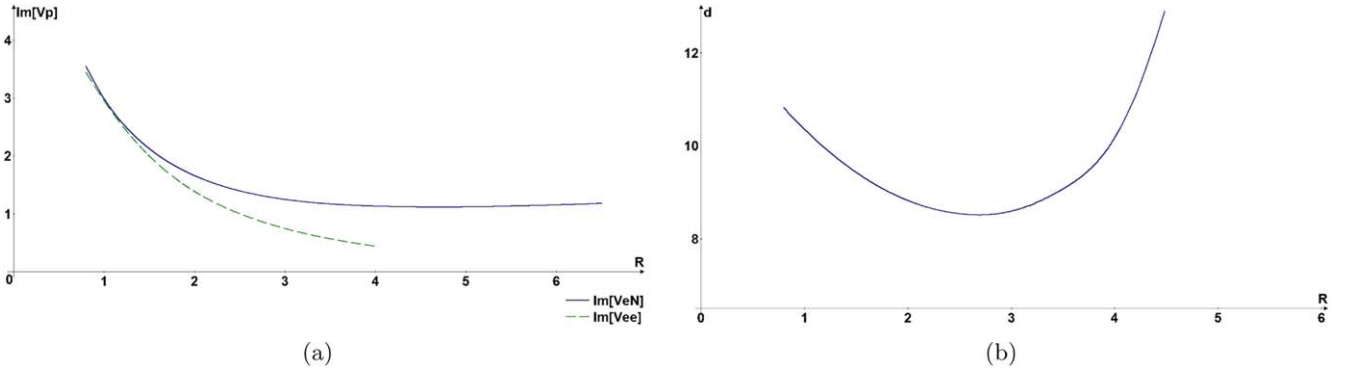


Figure 1. (a) Represents the dependence of the imaginary component of the \mathcal{P} -odd e -N and e - e matrix elements in the units of $10^{-5}G_F$ on the internuclear distance R in bohr (see equation (9)). (b) represents the dependence of the dipole moment matrix element in $10^{-5}ea_0$ on the internuclear distance R in bohr (see equation (9)). Figures 1(a) and (b) correspond to the case of mixing between $c^3\Pi_u$ and $X^1\Sigma_g^+$.

The final result for the nuclear spin-independent $E1^{\text{PNC}}$ amplitudes in the hydrogen molecule is as follows:

$$\begin{aligned} E1_{ee}^{\text{PNC}} &= \frac{1}{2} \sqrt{\frac{2J+1}{2J(J+1)}} 0.4 \cdot 10^{-10} G_F [\text{a.u.}] iea_0, \\ E1_{eN}^{\text{PNC}} &= \frac{1}{2} \sqrt{\frac{2J+1}{2J(J+1)}} 0.3 \cdot 10^{-10} G_F [\text{a.u.}] iea_0. \end{aligned} \quad (10)$$

Then, the parity nonconserving degrees for these effects now read

$$\begin{aligned} \mathcal{P}_{ee} &= \frac{1}{J(J+1)} 1.6 \cdot 10^{-17}, \\ \mathcal{P}_{eN} &= \frac{1}{J(J+1)} 1.2 \cdot 10^{-17}. \end{aligned} \quad (11)$$

From equations (10)–(11) it follows that for the hydrogen molecule the \mathcal{P} -odd e - e interaction effect is of the same order of magnitude and slightly larger than the \mathcal{P} -odd e -N one. Thus, in principle, it is possible to separate out the contribution of the PNC e - e interaction from the experimental data using our calculations, i.e. for the first time to manifest the existence of this kind of interaction in the low-energy regime. For this aim it suffices to mention that from any other atomic experiment on the NSI-PNC e -N interaction effect observation it is possible to extract the value of the weak charge Q_W . Then, using this value and calculation presented here one can extract the contribution of the NSI-PNC e - e interaction effect. Consequently the idea [14] about the enhancement of the \mathcal{P} -odd e - e interaction effect for the molecules is justified at least for H_2 . The homonuclear molecules with larger Z have a strong additional enhancement about Z^3 for the \mathcal{P} -odd e -N interaction effect. So in such molecules this effect strongly prevails over the e - e one, therefore the latter one cannot be separated out. We conclude that it is quite possible that H_2 is the only candidate for revealing the \mathcal{P} -odd e - e interaction in the low-energy regime and extracting the e - e interaction constant (which should be compared with the one obtained from the high energy experiments).

5. Theoretical simulation of the PNC experiment

In this section we present a theoretical simulation of a possible PNC experiment on the H_2 molecule, namely the observation of \mathcal{P} -odd rotation of the polarization plane of the light propagating through the vapor of H_2 molecules. The observable quantity is the rotation angle of the light polarization plane $\varphi_{\text{PNC}} \sim \text{Im}(E1^{\text{PNC}} \cdot M1)$. The total $E1^{\text{PNC}}$ amplitude that should be observed is equal to $E1^{\text{PNC}} = \frac{1}{2} \sqrt{\frac{2J+1}{2J(J+1)}} 0.7 \cdot 10^{-10} G_F [\text{a.u.}] iea_0$. Due to the rapid progress in the cavity-enhanced technique discussed in [28] and intracavity absorption spectroscopy (ICAS) experiments described in [29, 30] where a special construction of cavities allows to reach very large optical pathlength (to date up to 7×10^4 km) and to measure very accurately the optical rotation angles (to date up to the record birefringence phase-shift 3×10^{-13} rad), the observation of such a small \mathcal{P} -odd effect looks very promising in the future.

Now let us perform an estimate of the rotation angle φ_{PNC} . It is known that the value of optical pathlength is limited by the absorption of light in a medium. It is obvious that on resonance all light will be quickly absorbed. However the proposal [28] is based on the fact that it is possible to shift off-resonance where the \mathcal{P} -odd optical activity has its maximum and the absorption is small (see also [8]). The optical rotation angle increases linearly with the pathlength l , but the transmission of the light beam through the vapor defined by the Beer–Lambert law [31] falls as e^{-l/l_0} (l_0 is the absorption length). Then the PNC signal, i.e. the product of the rotation angle and the transmission function, is proportional to le^{-l/l_0} . The signal-to-noise ratio is optimal when $l = 2l_0$ [8, 32].

The PNC optical rotation angle is given by [8]:

$$\varphi_{\text{PNC}} = -\frac{4\pi l}{3\hbar c} \frac{\omega}{\Gamma_D} \frac{\rho}{2J+1} g(u, v) \langle gJv_1 || \mu || gJv_0 \rangle \text{Im}(E1^{\text{PNC}}), \quad (12)$$

where \hbar is the reduced Planck constant, c is the speed of light, ω is the resonant transition frequency, ρ is the number density of vapor. The Doppler width Γ_D is defined as [28]

$$\Gamma_D = \omega\beta(T), \quad (13)$$

where $\beta(T) = \sqrt{\frac{2k_B T}{Mc^2}}$ (k_B is the Boltzmann constant, T is the vapor temperature in Kelvin, M is the mass of a molecule). We define the Voigt profile for the resonant transition line function

$$\mathcal{F}(u, v) = \sqrt{\pi} e^{-(u+iv)^2} [1 - \text{Erf}(-i(u+iv))]. \quad (14)$$

In equation (14) $\text{Erf}(z)$ is the error function. The dimensionless variable u is defined as a ratio

$$u = \frac{\Delta\omega}{\Gamma_D}, \quad (15)$$

where $\Delta\omega$ is the detuning of the frequency. The dimensionless variable v is defined as a ratio

$$v = \frac{\Gamma}{2\Gamma_D}, \quad (16)$$

where Γ is the collisional broadening width and

$$\frac{\Gamma}{2} \sim \rho \sigma_{\text{col}} \beta(T) c, \quad (17)$$

where σ_{col} is the collisional cross-section. The refractive dependence of the profile is defined via

$$g(u, v) \equiv \text{Im } \mathcal{F}(u, v). \quad (18)$$

The absorption length is given by

$$l_0^{-1} = \frac{4\pi}{3\hbar c} \frac{\omega}{\Gamma_D} \frac{\rho}{2J+1} f(u, v) \langle gJv_1 || \mu || gJv_0 \rangle^2, \quad (19)$$

where

$$f(u, v) \equiv \text{Re } \mathcal{F}(u, v). \quad (20)$$

Since we are interested in off-resonance observation of the PNC effects (that is $u \gg 1$) the following asymptotics for $g(u, v)$ and $f(u, v)$ is applicable

$$\begin{aligned} g(u, v) &\approx \frac{1}{u}, \\ f(u, v) &\approx \frac{v}{u^2}. \end{aligned} \quad (21)$$

Now from the optimal signal condition $l = 2l_0$ one can express the number density ρ and then substitute this quantity in equation (12). As the result we obtain

$$\rho = \sqrt{\frac{3\hbar\beta^{1/2}(T)\omega u^2}{2\pi l \mu_N^2 \langle v_1 || g(R) || v_0 \rangle^2 J(J+1) \sigma_{\text{col}}}}, \quad (22)$$

$$\varphi_{\text{PNC}} = 0.7 \cdot 10^{-10} (G_F [\text{a.u.}]) \sqrt{\frac{\pi l \omega}{3\hbar c^2 \beta(T) \sigma_{\text{col}} J(J+1)}} e a_0. \quad (23)$$

Equation (23) was derived for the case of large J quantum numbers when it is possible to neglect the contribution of the E2 amplitude (see [16]). The expression for the optimal φ_{PNC} does not depend on the M1 amplitude but has the smallness $\sim 1/J$ (Note: however there is no benefit from choosing small J values since in this case the M1 transition will be suppressed by E2 transition which provides no PNC effect). Hence in our estimate we use $J \approx (28 - 30)$. The angle is

proportional to $\varphi_{\text{PNC}} \sim \beta^{-1/2}(T) \sim T^{-1/4}$ thus possible laser cooling of vapors can only very slightly improve the results. In our estimate the following values were used: rovibrational transition of interest with $\omega \approx 8 \times 10^{14} \text{ s}^{-1}$, the characteristic collision cross-section for H_2 $\sigma_{\text{col}} \approx 10^{-15} \text{ cm}^2$, $l = 7 \times 10^9 \text{ cm}$ [29]. This leads to the optimal PNC optical rotation angle

$$\varphi_{\text{PNC}} \sim 10^{-17} \text{ rad} \quad (24)$$

while the number density

$$\rho \sim 10^{17} \text{ cm}^{-3}. \quad (25)$$

Recall that the record birefringence phase-shift $3 \times 10^{-13} \text{ rad}$ has been recently measured [30]. Our estimate of the PNC rotation angle is by 4 orders of magnitude smaller than the record achievable in the experiment value. It is hardly believable also that the pathlength can be further increased ($\varphi_{\text{PNC}} \sim \sqrt{l}$). Concluding we can state that none of the recent ICAS experiments can provide at present a measurement of the PNC effects in the parahydrogen molecule, but in view of the rapid progress we have seen in ICAS such optical rotation angles may in the course of time be observed. Consequently, it would make it possible to reveal the weak electron-electron interaction at low-energies.

6. Conclusion

In this paper we put forward a proposal which may allow for the first time to observe directly the electron-electron weak PNC interaction in the low-energy regime. The parahydrogen molecule is the unique candidate for this purpose.

Our main goal of this paper was to demonstrate that the e - e PNC interaction can be directly observed in H_2 . For this purpose *ab initio* calculations of the corresponding effects were performed.

In the SLAC-E158 measurements the parity-violating asymmetry was measured to be $A_{PV} = -131 \pm 14(\text{stat}) \pm 10(\text{syst}) \times 10^{-9}$ [13]. Since the observed effect is roughly proportional to the factor $(1 - 4 \sin^2 \theta_W)$ (see equation (5)) which appears to be quite small, the accuracy of determination of $\sin^2 \theta_W$ from this experiment is better than 1%. The parahydrogen molecule H_2 is the unique molecular system where $G_{eN} = G_{ee}$ and hence the total weak interaction effect is also proportional to $(1 - 4 \sin^2 \theta_W)$ as in the SLAC-E158 experiment. If the cavity-enhanced technique will achieve the benchmark accuracy of about 10^{-17} rad then this can lead to very accurate determination of the Weinberg angle as well as revealing for the first time the electron-electron PNC interaction at low-energies.

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Appendix. Separation of the rotational part in the matrix elements of the $E1^{\text{PNC}}$ for ${}^3\Pi_u^-$ states

For our purposes it is convenient to perform calculations in the basis functions of (a) Hund’s coupling case. Case (b) basis functions can be expressed in terms of the (a) ones in the following way (see, e.g. [17]):

$$|\Lambda NSJ\rangle = \sum_{\Sigma=-S}^{+S} (-1)^{J-S+\Lambda} (2N+1)^{1/2} \times \begin{pmatrix} J & S & N \\ \Omega & -\Sigma & -\Lambda \end{pmatrix} |\Lambda S \Sigma J \Omega\rangle, \quad (\text{A1})$$

where Σ is the projection of the electronic spin momentum S on the internuclear axis. Consider the contribution of the ${}^3\Pi_u^- = \frac{1}{\sqrt{2}}(|\Lambda=1\rangle - |\Lambda=-1\rangle)$ to the PNC effects. Taking into account the fact that in the matrix element of the weak interaction $V_{\mathcal{P}}$ only the components with $\Omega=0$ survive, we perform the angular reduction and the transformation from the laboratory to the molecule-fixed frame ([18] and [17]) for the product of PNC and E1 matrix elements (see equation (4)):

$$\begin{aligned} & \langle g v_1 J M_J ({}^1\Sigma_g^+) | (\mathbf{d})_f | u_i v_j N_k J M_J'' ({}^3\Pi_u^-) \rangle \\ & \times \langle u_i v_j N_k J M_J'' ({}^3\Pi_u^- (0_u^-)) | V_{\mathcal{P}} | g v_0 J M_J' ({}^1\Sigma_g^+) \rangle \\ & = \sum_{M_J''} \langle g v_1 J M_J | (\mathbf{d})_f | u_i v_j N_k J M_J'' \rangle (-1)^{J-M_J'} \sqrt{2N_k+1} (2J+1) \\ & \times \begin{pmatrix} J & 1 & N_k \\ 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} J & 0 & J \\ -M_J' & 0 & M_J'' \end{pmatrix} \begin{pmatrix} J & 0 & J \\ 0 & 0 & 0 \end{pmatrix} \langle u_i v_j (0_u^-) | V_{\mathcal{P}} | g v_0 (0_g^+) \rangle \\ & = \langle g v_1 J M_J | (\mathbf{d})_f | u_i v_j N_k J M_J' \rangle (-1)^J \sqrt{2N_k+1} \\ & \times \begin{pmatrix} J & 1 & N_k \\ 0 & 1 & -1 \end{pmatrix} \langle u_i v_j (0_u^-) | V_{\mathcal{P}} | g v_0 (0_g^+) \rangle. \end{aligned} \quad (\text{A2})$$

Now we consider the E1 matrix element in equation (4). In order to separate out the rotational part one has to make the transformation to (a) Hund’s basis functions and the transformation from the laboratory to the molecule-fixed

frame [18]:

$$\begin{aligned} & \frac{1}{\sqrt{2}} (\langle g v_1 J M_J (\Lambda=0) | (\mathbf{d})_f | u_i v_j N_k J M_J' (S=1, \Lambda'=1) \rangle \\ & - \langle g v_1 J M_J (\Lambda=0) | (\mathbf{d})_f | u_i v_j N_k J M_J' (S=1, \Lambda'=-1) \rangle) \\ & = \frac{(-1)^J \sqrt{2N_k+1}}{\sqrt{2}} \sum_{\Sigma=-1}^{+1} \left(\begin{pmatrix} J & 1 & N_k \\ \Omega' & -\Sigma & -\Lambda' \end{pmatrix} \langle g v_1 J M_J | (\mathbf{d})_f | u_i v_j \Omega' J M_J' \rangle \right. \\ & \left. - \begin{pmatrix} J & 1 & N_k \\ \Omega'' & -\Sigma & -\Lambda'' \end{pmatrix} \langle g v_1 J M_J | (\mathbf{d})_f | u_i v_j \Omega'' J M_J' \rangle \right) \\ & = \frac{(-1)^{J-M_J} (2J+1) \sqrt{2N_k+1}}{\sqrt{2}} \begin{pmatrix} J & 1 & J \\ -M_J' & f & M_J \end{pmatrix} \sum_{\Sigma=-1}^{+1} \\ & \times \left(\begin{pmatrix} J & 1 & N_k \\ \Omega' & -\Sigma & -\Lambda' \end{pmatrix} \begin{pmatrix} J & 1 & J \\ 0 & -\Omega' & \Omega' \end{pmatrix} \langle g v_1 (\Omega=0) | (\mathbf{d})_f | u_i v_j \Omega' \rangle \right. \\ & \left. - \begin{pmatrix} J & 1 & N_k \\ \Omega'' & -\Sigma & -\Lambda'' \end{pmatrix} \begin{pmatrix} J & 1 & J \\ 0 & -\Omega'' & \Omega'' \end{pmatrix} \langle g v_1 (0_g^+) | (\mathbf{d})_f | u_i v_j \Omega'' \rangle \right). \end{aligned} \quad (\text{A3})$$

Note that $f = \Omega - \Omega'(\Omega'') = -\Omega'(\Omega'')$. The terms with $\Omega'(\Omega'') = 0, \pm 2$ vanish since corresponding 3j-symbols are set to zero. Since ${}^3\Pi_u^-$ and ${}^1\Sigma_g^+$ in parahydrogen possess only even rotational numbers then $N_k = J$. Now consider the interference contribution of M1 (equation (7)) and E1 transition amplitudes performing the summation over the projections of J and $f = q$:

$$\begin{aligned} 2M1^* \cdot E1_{{}^3\Pi_u^-} & = \frac{1}{3} \sqrt{\frac{2J+1}{J(J+1)}} \langle g J v_1 || \mu || g J v_0 \rangle^* \\ & \times (\langle g v_1 (0_g^+) | (\mathbf{d})_{-1} | u_i v_j (1_u) \rangle - \langle g v_1 (0_g^+) | (\mathbf{d})_{+1} | u_i v_j (-1_u) \rangle). \end{aligned} \quad (\text{A4})$$

Here we should note that the factor 1/3 originates from the interference of M1 and E1 matrix elements after angular reduction then it is more convenient to separate this factor out from their definition. Since we use adiabatic approximation, let us denote the electronic matrix elements as $d(R) = \langle g(0_g^+) | (\mathbf{d})_{-1} | u_i (1_u) \rangle - \langle g(0_g^+) | (\mathbf{d})_{+1} | u_i (-1_u) \rangle$ and $V_{\mathcal{P}}(R) = \langle u_i (0_u^-) | V_{\mathcal{P}} | g(0_g^+) \rangle$ (where R is the internuclear distance). Then substituting $N_k = J$ in equation (A2) we obtain the interference contribution of M1 and E1 ${}^{\text{PNC}}_{{}^3\Pi_u^-}$ transition amplitudes:

$$\begin{aligned} 2M1^* \cdot E1_{{}^3\Pi_u^-}^{\text{PNC}} & = \sqrt{\frac{2J+1}{2J(J+1)}} \langle g J v_1 || \mu || g J v_0 \rangle^* \\ & \times \sum_{ij} \left(\frac{\langle g v_1 | d(R) | u_i v_j \rangle \langle u_i v_j | V_{\mathcal{P}}(R) | g v_0 \rangle}{E_{g v_0} - E_{u_i v_j}} \right. \\ & \left. - \frac{\langle g v_1 | V_{\mathcal{P}}(R) | u_i v_j \rangle \langle u_i v_j | d(R) | g v_0 \rangle}{E_{g v_1} - E_{u_i v_j}} \right). \end{aligned} \quad (\text{A5})$$

Note that the minus sign in formulae (A5) is due to the imaginary matrix element $V_{\mathcal{P}}(R)$.

ORCID iDs

D V Chubukov  <https://orcid.org/0000-0002-0297-8083>

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