New Observables for Parity Violation in Atoms: Energy Shifts in External Electric Fields

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We consider hydrogen–like atoms in unstable levels of principal quantum number $n = 2$, confined to a finite size region in a non–homogeneous electric field carrying handedness. The interplay between the internal degrees of freedom of the atoms and the external ones of their c.m. motion can produce P–odd contributions to the eigenenergies. The nominal order of such shifts is $10^{-8}$ Hz. Typically such energy shifts depend linearly on the small P–violation parameters $\delta_i \simeq 10^{-12} \ (i = 1, 2)$, essentially the ratios of the P–violating mixing matrix elements of the $2S$ and $2P$ states over the Lamb shift, with $i = 1 \ (i = 2)$ corresponding to the nuclear spin independent (dependent) term. We show how such energy shifts can be enhanced by a factor of $\simeq 10^6$ in a resonance like way for special field configurations where a crossing of unstable levels occurs, leading to P–violating effects proportional to $\sqrt{\delta_i}$. Measurements of such effects can give information concerning the “spin crisis” of the nucleons.
In this article we deal with parity (P)–violating effects in atoms which are described in the standard model (SM) of elementary particle physics by the exchange of the Z–boson between the electrons in the shell and the quarks in the nucleus. There is a rich literature on this subject starting from the classical papers [1, 2]. For a review we refer to [3]. Experiments on P–violating effects in atoms have been done so far only with heavy atoms containing many electrons. Such experiments have given information on properties of the weak interactions and of the nuclei. The usefulness of this information has recently been demonstrated once again [4, 5].

Here we address the following question: Can one have real (complex) eigenenergies of stable (unstable) atomic states in external fields with a nontrivial dependence on the P–violating parameters? If this is possible, then one could determine the parameters of atomic P–violation by frequency measurements, which experimentally can be pushed to very high accuracy.

In the following we consider as an example the ordinary hydrogen atom $^1_1H$ in states with principal quantum number $n = 2$. In vacuum, and neglecting P–violation, the energy levels are $2P_{1\,2}, F = 0$; $2P_{1\,2}, F = 1$; $2S_{1\,2}, F = 0$; $2S_{1\,2}, F = 1$; $2P_{3\,2}, F = 1$; $2P_{3\,2}, F = 2$, with a degeneracy $2F + 1$, respectively. Here $F$ is the total angular momentum quantum number.

We denote the difference of the centers of the $2S_{1\,2}/2$ and $2P_{1\,2}/2$ energies, the Lamb shift, by $\tilde{A}_1$, the one of the $2P_{3\,2}/2$ and $2P_{1\,2}/2$ states by $\Delta$, and the hyperfine splittings by:

\[
\begin{align*}
\tilde{A}_1 &= E(2S_{1/2}, F = 1) - E(2S_{1/2}, F = 0), \\
\tilde{A}_2 &= E(2P_{1/2}, F = 1) - E(2P_{1/2}, F = 0), \\
\tilde{A}_3 &= E(2P_{3/2}, F = 2) - E(2P_{3/2}, F = 1)
\end{align*}
\]  

The values of these quantities and of the decay widths $\Gamma_S, \Gamma_P$ of the $S$ and $P$ states are experimentally well known [3] and theoretically well understood [7]. In the SM Z–boson exchange induces a P–violating contribution to the Hamiltonian, $H_{PV} = H_{PV}^{(1)} + H_{PV}^{(2)}$, where $H_{PV}^{(1)}(H_{PV}^{(2)})$ is the nuclear spin independent (dependent) contribution (for all our conventions and notations cf. [8]). This leads to a mixing of the states $2S_{1/2}, F$ and $2P_{1/2}, F$; $2P_{3/2}, F$, with the same $F$. Numerically this mixing is governed by two parameters $\delta_{1,2}$, essentially the ratios of the relevant matrix elements of $H_{PV}^{(1,2)}$ and the Lamb shift. To be precise, we define (cf. (3.17) of [8])

\[
\delta_i = -\frac{G}{64\pi} \sqrt{\frac{3}{2}} \frac{Q_{w}^{(i)}}{m_e r_B L}, \quad (i = 1, 2).
\]  

Here $G$ is Fermi’s constant, $r_B$ the Bohr radius and $Q_{w}^{(i)}$ are the weak charges of the proton. In the SM we have with $\theta_w$ the weak mixing angle

\[
\begin{align*}
Q_{w}^{(1)} &= 1 - 4 \sin^2 \theta_w, \\
Q_{w}^{(2)} &= -2(1 - 4 \sin^2 \theta_w)(\Delta u_p - \Delta d_p - \Delta s_p),
\end{align*}
\]  

where $\Delta q_p (q = u, d, s)$ are the quark contributions to the total proton spin. The difference $\Delta u_p - \Delta d_p = g_A$ is the well–known axial coupling constant of neutron $\beta$–decay and $\Delta s_p$ the spin contribution of $s$–quarks which is subject to great current
interest in connection with the so-called “spin crisis” of the nucleons \[9, 10\]. For a recent review cf. \[11\]. Numerically the constants \(\delta_i\) are very small:

\[
\begin{align*}
\delta_1 &= -4.91 \times 10^{-13}, \\
\delta_2 &= 1.23 \times 10^{-12}(1 - g_A^{-1}\Delta s_p).
\end{align*}
\]

For the numerics below we set \(\Delta s_p = 0\).

Let us now consider the hydrogen atom in a static external electric field \(E\). It has been discussed in detail in \[8\] that as a consequence of T–invariance, the energy levels of our atom in a spatially constant field (including the case of zero field, i.e. vacuum) get contributions from \(H_{PV}\) which are at most of order \(\delta_1, \delta_2, \delta_1\delta_2\), and thus extremely small.

We have now investigated atoms in spatially non–homogeneous external electric fields carrying handedness or chirality. We give a brief account of our results for \(^1\text{H}\) here. The detailed calculations will be published elsewhere \[12\]. We find that in a field with nonzero handedness energy levels – which are now due to an interplay of the internal motion and the c.m. motion of the atom – will in general get contributions linear in the parameters \(\delta_{1,2}\). For unstable states in special field configurations the complex energy eigenvalues get even contributions proportional to \(\sqrt{\delta_{1,2}}\).

As a specific example we discuss the situation of a hydrogen atom in a rectangular box with 3 segments \((\sigma = 1, 2, 3)\) and constant fields \(E^{(\sigma)}\) in the segments (Fig. 1). This situation is not quite realistic, since Maxwell’s equations require then charges on the interfaces of the segments. But for a demonstration of the principles of P–violating energy shifts this does not matter and the above situation is convenient to be analysed theoretically as a model for spatially “abrupt” changes of the fields. Spatially “adiabatic” changes of the fields will be discussed elsewhere \[13\].

We assume that we have a field \(E_3\), the same in all segments and pointing in 3–direction, and small additional fields \(E^{(\sigma)}\) \((\sigma = 1, 2, 3)\) which we treat as perturbations. An atom is assumed to move in such a field configuration inside the box. The fields in the box segments induce then Stark–mixings, but different ones in each segment.

Through the transition conditions for the wave function at the interfaces the internal and c.m. degrees of freedom of the atom get coupled. Then, the quasi–stationary states in the box, i.e. the states with single exponential decay, are complicated superpositions of all \(n = 2\) states with various wavefunctions for the c.m. motion. Now T–invariance is no longer powerful enough to exclude energy shifts proportional to \(\delta_{1,2}\). As an example we cite our results for the following values of the box size and of the electric fields:

\[
A_1 = A_2 = A_3 = 8 \text{ nm},
\]

\[
R_1^{(1)}/A_1 = 0.45, \quad R_1^{(2)}/A_1 = 0.55.
\]

Here, the \(A_i, i = 1, 2, 3\) denote the total lengths of the the box in 1-, 2- and 3–direction respectively and the \(R_1^{(\sigma)}\) determine the widths of segments \(S^{(\sigma)}\) \((\sigma = 1, 2, 3)\), which are defined through

\[
S^{(\sigma)} := \{\mathbf{R} = (R_1, R_2, R_3) \mid R_1^{(\sigma - 1)} < R_1 < R_1^{(\sigma)}, \ 0 < R_2 < A_2, \ 0 < R_3 < A_3\}
\]
\((R_1^{(0)} := 0, R_1^{(3)} := A_1)\). For the electric fields we take as an example where the effect is “large”:

\[
\begin{align*}
\mathcal{E} &= 340 \text{V/cm}, \\
\mathcal{E}'^{(\sigma)} &= \mathcal{E}' \eta^{(\sigma)},
\end{align*}
\]

with

\[
\mathcal{E}' = 84 \text{V/cm},
\]

\[
\eta^{(1)} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \eta^{(2)} = 0, \quad \eta^{(3)} = \begin{pmatrix} 0 \\ 0.5 \\ 0 \end{pmatrix}.
\]

We calculate then as observables for P–violation the differences of energies of corresponding levels in the above electric field configuration \(\mathcal{E}\mathbf{e}_3 + \mathcal{E}'^{(\sigma)}\) and in \(\mathcal{E}\mathbf{e}_3 + \mathcal{E}'_R^{(\sigma)}\) obtained by a reflection \(R\) on the plane \(x_2 = A_2/2\):

\[
R : \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \mapsto \begin{pmatrix} x_1 \\ A_2 - x_2 \\ x_3 \end{pmatrix}.
\]

Of course, this reflection just means a sign change in \(\eta^{(2)}_e\) in \((11)\). In this way we obtain for the lowest level which evolves continuously from the vacuum level \(2S_{1/2}, F = 1, F_3 = 1\), as the confinement in the box and the fields are turned on, the following result:

\[
\begin{align*}
\Re(E(\mathcal{E}, \{\mathcal{E}'^{(\sigma)}\}) - E(\mathcal{E}, \{\mathcal{E}'_R^{(\sigma)}\})) / \hbar &= \left(2.4 \delta_1 - 40.4 \delta_2 + \mathcal{O}([\mathcal{E}'/\mathcal{E}]^3)\right) \text{kHz,} \\
\Im(E(\mathcal{E}, \{\mathcal{E}'^{(\sigma)}\}) - E(\mathcal{E}, \{\mathcal{E}'_R^{(\sigma)}\})) / \hbar &= \left(-2.2 \delta_1 + 17.3 \delta_2 + \mathcal{O}([\mathcal{E}'/\mathcal{E}]^3)\right) 10^4 \text{s}^{-1}
\end{align*}
\]

The coefficients of the parameters \(\delta_i\) were calculated in perturbation theory up to second order in \(\mathcal{E}'/\mathcal{E}\).

We thus have demonstrated the existence of P–violating energy shifts linear in \(\delta_{1,2}\). But from \((13)\) we see that these shifts are still small, of order \(10^{-8}\) Hz (cf. \((1)\)), and presumably hard to measure. We will show now that there exists the possibility of having much bigger P–violating energy shifts proportional to \(\sqrt{\delta_{1,2}}\). To see this, consider the two states \(2S_{1/2}, F = 1, F_3 = \pm 1\) in vacuum in the absence of P–violation, i.e. for \(\delta_1 = \delta_2 = 0\). These states are unstable and have the same complex energy eigenvalue. Let us now “turn on” the confinement in the box, the P–violation and the zero order electric field \(\mathcal{E}\mathbf{e}_3\). It can be shown \((12)\) that T–invariance still guarantees a twofold degeneracy of the complex eigenenergies for the states evolving from the above ones at \(\mathcal{E} = 0, \delta_{1,2} = 0\). Turning on the fields \(\mathcal{E}'^{(\sigma)} (\sigma = 1, 2, 3)\), we lift, in general, this degeneracy and obtain two distinct levels. But we can search for values of \(\mathcal{E}'^{(\sigma)} \neq 0\) where these two levels cross again if \(\delta_1 = \delta_2 = 0\). The crossing must be in the real and imaginary parts of the complex energy levels. The calculation is performed using convenient versions of degenerate perturbation theory (in the \(\mathcal{E}'^{(\sigma)}\)–couplings of the atom) (cf. \((12, 14, 15)\)). Since we are dealing with unstable states we typically get a non–hermitian \(2 \times 2\) matrix \(\mathcal{H}\) (cf. \((12)\)), whose complex eigenvalues are the sought
energies. The structure of this matrix is again restricted by T–invariance to be of the form
\[ \tilde{\mathcal{H}} = \begin{pmatrix} \tilde{H}_{++} & \tilde{H}_{+-} \\ \tilde{H}_{-+} & \tilde{H}_{--} \end{pmatrix} \] (14)
with \( \tilde{H}_{++} = \tilde{H}_{--} \). Then the eigenvalues are
\[ E_\pm = \tilde{H}_{++} \pm \sqrt{\tilde{H}_{+-} \tilde{H}_{-+}}. \] (15)
Expanding the matrix elements \( \tilde{H}_{m'm} \) in powers of \( \delta_1, \delta_2 \) we have
\[ \tilde{H}_{m'm} = \tilde{H}_{m'm}^{(0)} + \delta_1 \tilde{H}_{m'm}^{(1)} + \delta_2 \tilde{H}_{m'm}^{(2)} + \ldots, \] \((m', m \in \{ +1, -1 \})\). (16)
For a non–hermitian matrix \( \tilde{\mathcal{H}} \) we can have
\[ \tilde{H}_{++}^{(0)} = 0, \]
\[ \tilde{H}_{+-}^{(i)} \neq 0, \quad i = 1, 2, \]
\[ \tilde{H}_{-+}^{(0)} \neq 0. \] (17)
This gives
\[ E_\pm = \tilde{H}_{++}^{(0)} \pm \sqrt{\sum_{i=1}^{2} \delta_i \tilde{H}_{+-}^{(i)} \tilde{H}_{-+}^{(i)}} + \mathcal{O}(\delta_1, \delta_2). \] (18)
We found that the conditions (17) are fulfilled for instance for a zero order field \( \mathcal{E} = 100 \) V/cm and fields \( \mathcal{E}'^{(s)} =: \mathcal{E}' \eta^{(s)} \) with
\[ \eta^{(1)} = \begin{pmatrix} 3.91 \\ 0.0764 \\ 0 \end{pmatrix} + \mathcal{O}(\mathcal{E}'/\mathcal{E}) \]
\[ \eta^{(2)} = 0 \]
\[ \eta^{(3)} = \begin{pmatrix} 3.91 \\ -0.328 \\ 0 \end{pmatrix} + \mathcal{O}(\mathcal{E}'/\mathcal{E}) \] (19)
The higher order terms are under control for \( \mathcal{E}' < 5 \) V/cm, i.e. they can shift the “magic” values of \( \eta^{(s)} \) (18) only slightly.
In Figs. 2a, b we show the resulting behaviour of the real and imaginary parts of \( E_\pm (\mathcal{E}'^{(s)}) - E_\pm (\mathcal{E}'_R^{(s)}) \) as a function of the 2nd component of the electric field in the 3rd segment, \( \mathcal{E}_2^{(s)} = \mathcal{E}' \eta_2^{(s)} \), keeping all other field components fixed, i.e. we vary only \( \eta_2^{(s)} \). We see from (18) that for \( \mathcal{E}' = 5 \) V/cm, the “magic” value is
\[ \mathcal{E}_2^{(s)}_{\text{res}} = -1.638 \cdot (1 + \mathcal{O}(\mathcal{E}'/\mathcal{E})) \) V/cm. (20)
P–violation induces a sharp “resonance” at \( \mathcal{E}_2^{(s)} = \mathcal{E}_2^{(s)}_{\text{res}} \) where the P–violating energy shift is enhanced by six orders of magnitude. The width of the peak is proportional to
and found to be $2.6 \cdot 10^{-12} \text{V/cm}$. Note, however, that in Figs. 2a, b the differences of the real parts of the energies of the levels are at maximum of the order of $10^{-5} \text{Hz}$ whereas the lifetime of the levels is calculated to be $4.13 \cdot 10^{-8} \text{s}$. This corresponds to a line width $\Delta E/h = 3.86 \cdot 10^6 \text{Hz}$. Thus it is certainly not an easy task to detect frequency shifts of order $10^{-5} \text{Hz}$ in such broad lines. But our example is only meant to provide an illustration how energy shifts proportional to $\sqrt{\delta_{1,2}}$ can be obtained. No effort has been made here to optimize the effect for a realistic experimental situation.

To conclude: In this paper we have demonstrated that the eigenenergies of a hydrogen atom in a spatially inhomogeneous electric field with nonzero chirality get in general contributions linear in the P–violation parameters $\delta_{1,2}$ (2). This statement is valid both for stable and unstable states and, of course, easily extended to other atoms. To measure such P–violating contributions to eigenenergies one would look at the difference of their values for a given electric field configuration and its spatially reflected one. For special electric field configurations with nonzero handedness where two unstable levels have the same complex eigenenergy in the absence of P–violation, we can obtain large P–violating energy shifts proportional to $\sqrt{\delta_{1,2}}$. The comparison of the two levels at the crossing point with the levels for the field configuration of opposite handedness should show a drastic difference: Under a reversal of the handedness the P–violating shift gets multiplied by a phase factor $i$. This means that the shifts in the real and imaginary parts of the complex eigenenergies are exchanged. Finally we note that for the case of hydrogen discussed here all our energy shifts are much more sensitive to the parameter $\delta_2$ than to $\delta_1$ (cf. (1–3)). The reason for this is the same as given in (6.1), (6.2) of [8]. Thus a measurement of our effects could lead to a determination of the nuclear spin–dependent weak charge $Q_{\text{W}}^{(2)}$ (3) which depends on the contribution of s–quarks to the proton spin. In this way parity violation in atoms could give information concerning the “spin crisis” of the nucleons.

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Fig. 1. Sketch of the electric field configuration in a box divided into three segments (1)–(3). The electric field is homogeneous within every segment and varies suddenly along the 1–direction at the interfaces.
Fig. 2. The decadic logarithm of the absolute values of the real (a) and imaginary (b) parts of the P-violating energy-difference $E_\pm(\mathcal{E}^{(s)}) - E_\pm(\mathcal{E}^{(s)}_R)$ (18) vs. the deviation $\mathcal{E}_2^{(3)} - \mathcal{E}_{2,\text{res}}^{(3)}$ from the resonance value (20) for which the P-even splitting of levels is removed, revealing a P-violating splitting of the order of $\sqrt{\delta_{1,2}}$. 