Proton Polarization Shifts in Electronic and Muonic Hydrogen

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Abstract

The contribution of virtual excitations to the energy levels of electronic and muonic hydrogen is investigated combining a model-independent approach for the main part with quark model predictions for the remaining corrections. Precise values for the polarization shifts are obtained in the long-wavelength dipole approximation by numerically integrating over measured total photoabsorption cross sections. These unretarded results are considerably reduced by including retardation effects in an approximate way since the average momentum transfer (together with the mean excitation energy) turns out to be larger than usually assumed. Transverse and seagull contributions are estimated in a simple harmonic oscillator quark model and found to be non-negligible. Possible uncertainties and improvements of the final results are discussed.

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1. There has been tremendous progress in the laser spectroscopy of hydrogen and deuterium atoms \[1\] which now are even sensitive to small nuclear and proton structure effects. One of these - traditionally the least understood - is the virtual excitation of the nucleus which acts back on the bound lepton. While the effect in deuterium is comparatively large and has been evaluated theoretically with increasing sophistication and reliability \[2\], the proton polarization shifts have not received much attention up to now. Khriplovich and Sen’kov \[3\] have estimated the shift in the electronic $1S$-state as $-71 \pm 11 \pm 7$ Hz using values for the static proton polarizabilities and assuming a mean excitation energy of $\sim 300$ MeV. They attribute the quoted errors to the use of a relativistic approximation for the electron and to the experimental values of the polarizabilities. However, experience gained in many decades of nuclear polarization calculations has told us that the use of an average excitation energy (the “closure approximation”) can be a considerable source of uncertainty unless one calculates it precisely. In addition, one has to make sure that other ingredients to the polarization shift (higher multipoles, transverse excitations) are well under control before a definite answer can be given. It is the purpose of this note to re-evaluate the polarization shift without the questionable use of a mean excitation energy and other simplifying assumptions. Since an experiment is in progress at PSI to measure the Lamb shift in muonic hydrogen \[4\] we will also evaluate the polarization shift for this case. Actually, with the experimental accuracies achievable in the near future, it turns out that the proton polarization shifts are of much greater importance for muonic than for electronic hydrogen.

2. For light electronic and muonic atoms the energy shift due to virtual excitations can be written as an integral over the forward virtual Compton amplitude. This quantity in turn may be expressed by its imaginary part, i.e. the structure functions $W_{1/2}(\nu, Q^2)$ which are measurable in the inclusive reaction $e + p \rightarrow e’ + X$. In the absence of detailed experimental information for all relevant values of momentum transfer $Q$ and energy transfer $\nu$ it is customary to apply the long wavelength (or unretarded dipole) approximation which should be valid for $\bar{Q} \langle r^2 \rangle^{1/2} \ll 1$ where $\langle r^2 \rangle^{1/2}$ is the root-mean-square radius of the proton and $\bar{Q}$ an average momentum transfer. In this limit it is possible to express the structure functions by the experimentally measured photoabsorption cross section $\sigma_\gamma(\nu)$. Bernabéu and Ericson have derived in this way the following expression for the energy shift \[5\]

$$\Delta E_{nl} = -\frac{\alpha}{2\pi^2} \frac{m}{m} \left| \psi_{nl}(0) \right|^2 \int_0^\infty d\nu \sigma_\gamma(\nu) f \left( \frac{\nu}{2m} \right)$$

with

$$f \left( \frac{\nu}{2m} \right) = \frac{8m^2}{\pi} \int_0^\infty dQ^2 \frac{1}{Q^2} \int_0^Q d\xi \sqrt{Q^2 - \xi^2} \frac{Q^2 + 2\xi^4/Q^2}{(\nu^2 + \xi^2)(Q^4 + 4m^2\xi^2)}.$$
accuracy. We first note that it is possible to perform all integrations in eq. (2) and to obtain
\[ f(x) = -2 - 2 \ln(4x) + \frac{1 + 2x^2}{x^2} \left[ \sqrt{x^2 + x} \ln \frac{\sqrt{x^2 + x} + x}{\sqrt{x^2 + x} - x} + g(x) \right] \] (3)
with
\[ g(x) = \sqrt{|x^2 - x|} \left[ \Theta(1 - x) \frac{2 \arctan \frac{\sqrt{x^2 - x}}{x}}{x} - \Theta(x - 1) \ln \frac{x + \sqrt{x^2 - x}}{x - \sqrt{x^2 - x}} \right] . \] (4)
The function \( f(x) \) has quite different limits for small and large arguments:
\[ f(x) \rightarrow \pi x^{-3/2} \quad \text{for } x \rightarrow 0 \] (5)
\[ f(x) \rightarrow \left. \frac{5}{4x^2} \left( \ln(4x) + \frac{19}{30} \right) \right|_{x \rightarrow 0} \quad \text{for } x \rightarrow \infty \] (6)
which makes a crucial difference between nuclear polarization shifts, say, in muonic deuterium and in electronic hydrogen. Krhrilovich and Sen’kov have only retained the leading logarithm in eq. (3) which is justified considering the much greater error which comes from pulling out the logarithmic term evaluated at the excitation energy of the \( \Delta(1232) \) and expressing the remaining integral in terms of the sum of polarizabilities
\[ \bar{\alpha} + \bar{\beta} = \frac{1}{2\pi^2} \int_0^{\infty} d\nu \frac{\sigma_\gamma(\nu)}{\nu^2} . \] (7)

3. In view of the well-known deficiencies of the closure approximation we have decided to evaluate the polarization shift by integrating numerically over the experimentally measured photon absorption cross section. We have taken the recent Mainz data from \( \nu = 200 - 800 \) MeV, the older Daresbury data from \( \nu = 800 - 4215 \) MeV and the parametrization \( \sigma_\gamma(\nu) = 96.6 \mu b + 70.2 \mu b \text{ GeV}^{1/2}/\sqrt{\nu} \) above 4215 MeV. Below 200 MeV four angular distributions in \( \gamma p \rightarrow \pi^- n \) (from Fig. 1 in ref. [9]) have been converted to total cross sections and the threshold behaviour has been parametrized as \( \sigma_\gamma(\nu) = 18.3 \mu b \text{ MeV}^{-1/2}\sqrt{\nu - \nu_{th}} \). The numerical integration was done by simple Simpson integration over linearly interpolated data points and the whole procedure was checked by evaluating eq. (7). We obtained
\[ \bar{\alpha} + \bar{\beta} = 13.75 \cdot 10^{-4} \text{ fm}^3 \] (8)
in good agreement with a recent analysis [10] but smaller than the value \( 14.2 \cdot 10^{-4} \text{ fm}^3 \) used in Ref. [3]. This is due to the fact that the older cross sections which have been analysed in Ref. [1] are systematically higher than the new Mainz data.

The \textit{unretarded} results for the electronic (e) and muonic (\( \mu \)) polarization shifts are then
\[ \Delta E_{nS}^e = -106.5 \frac{\text{Hz}}{n^3} \] (9)
\[ \Delta E_{nS}^\mu = -202 \frac{\mu eV}{n^3} . \] (10)

\footnote{This has also been noted before [3].}
In view of the small electron mass it is not surprising that the relativistic approximation (including the constant term) agrees with the exact result to more than 4 digits. Equation (9) is larger than the estimate of ref. [3] because the integral over virtual excitations gets contributions well above the ∆-resonance. This can be easily seen from any graph of the total photoabsorption cross section versus photon energy but made more quantitative by asking for the value of the mean excitation energy $\bar{\nu}$ which – when substituted into the logarithm of eq. (8) – gives the same result for the shift. We find $\bar{\nu} \simeq 410$ MeV both for electronic and muonic hydrogen. Therefore predictions assuming that only the ∆ isobar contributes to virtual excitations of the proton [12] are not very reliable. In the muonic case the approximation (6) still gives more than 96% of the exact numerical result whereas the non-relativistic approximation (5) overestimates it by more than 40%. This is, of course, consistent with the fact that the mean excitation energy is nearly four times larger than the muon mass.

4. The large value of the mean excitation energy also casts some doubt on the use of the unretarded dipole approximation. For example, in a simple constituent harmonic oscillator quark model one naively expects an associated mean momentum transfer of $\bar{Q} \simeq \sqrt{M_{\text{quark}}\bar{\nu}} \simeq 350$ MeV. This will have an appreciable effect when inserted in the elastic form factor which, e.g. in the dipole approximation is given by $F_0(Q^2) \simeq 1/(1+Q^2/Q_0^2)^2$ with $Q_0^2 = 0.71$ GeV$^2$. Inelastic transition form factors to low-lying resonances have approximately the same $Q$-dependence apart from threshold factors which are characteristic for the specific angular momentum of the resonance (see below for a non-relativistic example). Therefore one obtains a rough estimate for the effect of retardation when the square of the elastic form factor $F_0^2(Q^2)$ is inserted in the $Q^2$-integral of eq. (4). Instead of the dipole form factor we have employed a more realistic parametrization of the charge form factor of the proton given in eq. (9) and table 3 of ref. [13]. A careful numerical evaluation of the remaining double integral then gives for the retarded polarization shifts

$$\Delta E_{nS}^e = -\frac{88.9}{n^3} \text{ Hz} \quad (11)$$

$$\Delta E_{nS}^\mu = -\frac{112}{n^3} \mu\text{eV}. \quad (12)$$

Use of the dipole form factor changes the numerical values to 89.3 and 114 for electron and muon, respectively. Equation (11) is nearly 20% smaller in magnitude than the unretarded result and the polarization shift in muonic hydrogen gets almost halved due to retardation effects. This reduction can be translated into a mean momentum transfer which – when inserted into the square of the elastic form factor – cuts the unretarded values by just this amount. In this way one obtains $\bar{Q} \simeq 180$ and 340 MeV/c for the electronic and muonic case respectively.

5. At present this seems to be the best model-independent estimate for the polarization shifts in hydrogen but it still neglects higher multipoles and relies on a standard but not very well tested procedure to correct the unretarded dipole approximation. Contrary to the deuteron case where excellent potential models are available, a reliable (relativistic) model of the nucleon does not
exist to calculate all these contributions. Here we take the simple non-relativistic harmonic oscillator quark model to estimate them. In this model it is easy to evaluate analytically the longitudinal (inelastic) structure function

\[ S_L(\nu, q) = \sum_{N=1}^{\infty} \delta \left( \nu - N\omega - \frac{q^2}{6M_{\text{quark}}} \right) \frac{y^N}{N!} e^{-y} \]  

(13)
as well as the transverse one\footnote{The structure functions $S_{L/T}$ are linear combinations of the usual $W_{1/2}$ and are more convenient in the framework of ref. \cite{14} which uses the energy transfer $\nu$ and the three-momentum transfer $q \equiv |q|$ as variables whereas ref. \cite{16} employs the invariants $\nu$ and $Q^2$.}

\[ S_T(\nu, q) = \frac{q^2}{2M_{\text{quark}}^2} S_L(\nu, q) + \frac{2\omega}{3M_{\text{quark}}} \sum_{N=1}^{\infty} \delta \left( \nu - N\omega - \frac{q^2}{6M_{\text{quark}}} \right) \frac{y^{N-1}}{(N-1)!} e^{-y} \]  

(14)

Here $y = (qb)^2/3$ where $b$ is the oscillator length and $\omega = 1/(M_{\text{quark}}b^2)$ the harmonic oscillator frequency. In this model the excitation spectrum consists of sharp lines at $N\omega$ shifted by the recoil energy of the proton and the elastic form factor is gaussian ($F_0^2(q) = \exp(-y)$) so that the proton rms radius is directly given by the oscillator length $b$. It should be noticed that the first and the second term in eq. (14) come from excitations by the spin and the convection current, respectively. Note also that the above structure functions fulfill Siegert’s theorem $\lim_{q \to 0} S_L(\nu, q)/q^2 = \lim_{q \to 0} S_T(\nu, q)/(2\nu^2) = \sigma_\gamma(\nu)/(4\pi^2\alpha\nu)$ and that all excitations are indeed multiplied by the square of the elastic form factor. In the low-$q$ limit the first excited state exhausts the dipole absorption cross section which is not a very realistic feature of the model. Other shortcomings are the well-known inability\footnote{The structure functions $S_{L/T}$ are linear combinations of the usual $W_{1/2}$ and are more convenient in the framework of ref. \cite{14} which uses the energy transfer $\nu$ and the three-momentum transfer $q \equiv |q|$ as variables whereas ref. \cite{16} employs the invariants $\nu$ and $Q^2$.} of the harmonic oscillator quark model to reproduce both the empirical rms-radius ($\langle r^2 \rangle^{1/2} = 0.86$ fm ) and the polarizabilities of if the constituent quark mass is fixed to $M_{\text{quark}} = M_{\text{proton}}/3$. We also make this choice because the masses of the constituents should add up to the total mass in a consistent non-relativistic treatment. In addition, this value gives the correct recoil energy and leads to a reasonable result for the magnetic moment of the proton. This leaves only the harmonic oscillator length as free parameter which we have fixed in such a way that the results from the unretarded dipole approximation are obtained. In this way the quark model results can be directly compared with the shifts evaluated in the model-independent approach. It is quite obvious that a non-relativistic model becomes inadequate for excitation energies and momenta of the order of the constituent mass. However, here our aim only is to obtain a rough estimate for the remaining corrections beyond the retarded dipole approximation and for this purpose the harmonic oscillator quark model may be not totally useless.

To obtain a quantitative estimate we have inserted the analytic expressions (13, 14) into the formulae in the Appendix of ref. \cite{14} (which keep the relativistic kinematics for the lepton), summed over oscillator shells up to $N_{\text{max}} = 20$ and integrated numerically over the momentum transfer up to $q_{\text{max}} = 3000$ MeV. Special care has to be exercised because of the apparent singularity in the transverse weight function at $q = 0$ which is canceled by the seagull contribution. The latter one is required for a gauge-invariant treatment of non-relativistic systems.
Other numerical difficulties arise from the very different scales of electron mass and mean excitation energy which requires very high numerical accuracy (up to $60 \times 72$ gaussian points compared to $6 \times 72$ in the muonic case) and from the slow convergence ($\sim 1/N_{\text{max}}^2$) of the sum over excitations for the spin current which peaks at high momentum, i.e. high $N$. The latter problem has been overcome by an analytic resummation and the overall numerical stability has been checked by varying $q_{\text{max}}$, $N_{\text{max}}$ and the number of gaussian integration points. The results of the calculation are collected in Table 1. As expected the $b$-values are too small to account for the proton radius while the $\omega$-values ($\sim 280$ MeV) seem reasonable for low-lying nucleonic excitations. A simple way to cure these deficiencies is to attribute the gaussian form factor to the quark core and to introduce an extra formfactor $1/(1 + \beta^2 q^2)$ for the meson cloud which surrounds the core and brings the rms-radius of the model in agreement with the experimental value $[16]$. Although this is rather ad hoc and theoretically not very appealing we have included this variant also in Table 1. Note that the unretarded dipole approximation (and therefore the value obtained in ref. $[3]$) also includes some transverse excitations: eq. (6) would read $(\ln 4x + 1)/x^2$ if only longitudinal excitations are kept. While the longitudinal excitations (including all multipolarities) are seen to dominate, virtual transverse excitations induced by the currents cannot be neglected since the mean momentum transfer is of the order of the constituent quark mass. This is particularly important for the spin current in muonic hydrogen because its contribution grows with momentum transfer.

|                               | electronic hydrogen $[\text{Hz}]$ | muonic hydrogen $[\mu\text{eV}]$ |
|-------------------------------|----------------------------------|----------------------------------|
|                               | (A)                              | (B)                              |
| unretarded dipole (input)     | - 106.4                          | - 201.8                          |
| retarded dipole               | - 94.3                           | - 131.6                          |
| full longitudinal             | - 78.2                           | - 120.2                          |
| spin current                  | - 7.2                            | - 39.1                           |
| convection current + seagull  | - 19.2                           | - 16.9                           |
| total                         | - 104.6                          | - 176.2                          |
| correction to retarded dipole | - 10.3                           | - 44.6                           |
|                               | - 6.5                            | - 24.0                           |

Table 1: Polarization shifts to the 1S level in electronic and muonic hydrogen evaluated in the harmonic oscillator quark model. The parameters ($M_{\text{quark}} = 312.8$ MeV, $b = 0.657$ fm for electronic hydrogen, $b = 0.674$ fm for muonic hydrogen) have been fitted to give the unretarded
dipole approximation and the corresponding results are given under the heading (A). In case (B) an additional meson-cloud form factor has been introduced to reproduce the experimental proton radius.

The ad-hoc introduction of the meson-cloud form factor reduces all contributions and brings the retarded dipole approximation more in accord with the calculation employing realistic form factors.

6. In conclusion, we have evaluated the proton polarization shifts in electronic and muonic hydrogen in a fairly model-independent way by integrating over the experimental photoabsorption cross section and accounting for retardation by use of the empirical elastic form factor. The remaining contributions (mostly from transverse excitations) have been estimated in a simple harmonic oscillator quark model and are therefore rather model-dependent and uncertain. Since it is physics in the resonance region which dominates these contributions, the theoretical situation will probably remain so unless better experimental information from inclusive \( ep \) -scattering in this region is available. For our final values we add the corrections (B) listed in Table 1 to eqs. (11, 12) and assign an error to them which covers the values obtained in case (A). This seems reasonable and prudent in view of the mentioned uncertainties and the inadequacy of the harmonic oscillator quark model. In addition, we take the difference between the retarded dipole result obtained with realistic form factors and the one with the gaussian form factor for the core and monopole form factor for the meson cloud as error estimate for the model-independent contribution. Adding the errors linearly we obtain in this way our final result for the polarization shifts

\[
\Delta E_{nS}^e = -\frac{95 \pm 7}{n^3} \text{ Hz} \quad (15)
\]

\[
\Delta E_{nS}^\mu = -\frac{136 \pm 30}{n^3} \mu\text{eV} \quad (16)
\]

The first value is one order of magnitude below the present experimental accuracy (840 Hz) in the \( 2S - 1S \) transition \( \text{[1]} \) whereas the planned Lamb shift experiment in muonic hydrogen \( \text{[3]} \) aims for a precision which is comparable to the uncertainty in \( \Delta E_{2S}^\mu \). Incidentally, the proton polarization contribution to this Lamb shift has nearly the same magnitude as the hadronic vacuum-polarization correction \( \text{[17]} \) which, however, is more precisely known. A more accurate evaluation of the former contribution is therefore needed for a better determination of the proton radius from the muonic Lamb shift experiment.

Note added: After submission of the manuscript additional calculations of the muonic polarization shift using different methods have been reported. Faustov and Martynenko \( \text{[18]} \) obtain nearly the same value as reported in this paper whereas Pachucki’s number \( \text{[19]} \) is slightly lower.

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