Deuteron nuclear polarization shifts with realistic potentials

W. Leidemann
European Centre for Theoretical Nuclear Physics and Related Areas, Villa Tambosi, I-38050 Villazzano (Trento), Italy

R. Rosenfelder
Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland
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We calculate the second-order corrections to the atomic S-level shifts in electronic and muonic deuterium due to virtual excitations of the deuteron using wave functions from realistic potentials. Common approximations like the long-wavelength limit or the closure approximation are avoided by integrating over the inelastic structure functions of the deuteron with specified weight functions. Transverse excitations are also included consistently. We estimate the potential dependence of our numerical results to be less than 2%.

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Recent experimental progress in measuring S-level transitions in electronic hydrogen and deuterium [1, 2] has reached a precision where the virtual excitation of the deuteron cannot be neglected anymore. These experiments can be either used to test QED in bound systems or to measure the shift due to the finite size of the deuteron. In addition, planned experiments at PSI [3] will need precise theoretical predictions for the nuclear polarization shifts in muonic deuterium in order to extract the charge radius of the deuteron with the highest possible accuracy. The latter quantity is of considerable interest: Some time ago it was noted [4] that the nucleon-nucleon triplet scattering length and the experimental value of the charge radius of the deuteron are not on the linear curve predicted by nearly all potential models [5, 6]. However, there is an inconsistency between the low-momentum transfer data of Ref. [7] on which the experimental value of the deuteron charge radius is based and the higher momentum transfer data from Ref. [8] in the region of overlap. Thus the question of the precise value of the deuteron charge radius is not settled at present [9].

We will concentrate on S-level shifts because the nuclear polarization shifts in higher orbits (where the lepton does not penetrate the nucleus) are much smaller and can be estimated with sufficient accuracy by knowing the electric dipole polarizability of the target. Previously the nuclear polarization shift in the deuteron was calculated with wave functions from simple separable potentials, like those of Yamaguchi and Tabakin [10].

It is the purpose of this paper to report the results of a detailed calculation which employs state-of-the-art phenomenological NN potentials, namely, the Paris, Nijmegen, Argonne (AV14), and Bonn potentials. We use the formalism of Ref. [11] where the nuclear polarization shift in $l = 0$ states of light atoms is expressed in terms of the forward Compton amplitude. The Coulomb gauge is employed in the following but the total nuclear polarization shift is gauge invariant if the nuclear currents are conserved and the gauge condition for the two-photon amplitude [12] is fulfilled. The longitudinal (L) and transverse (T) parts of the forward Compton amplitude are then expressed by their imaginary parts where the "sea gull" term acts as a subtraction constant in the dispersion relation for the transverse amplitude. In this way the nuclear polarization shift is obtained as an integral over the inelastic structure functions $S_{L/T}(q,\omega)$ of the target:

$$\Delta\epsilon_{n0} = -\,8\alpha^2 R_{n0}\,|\phi_{n0}(0)|^2 \int_0^\infty dq \int_0^\infty d\omega\,[K_L(q,\omega)\,S_L(q,\omega) + K_T(q,\omega)\,S_T(q,\omega) + K_S(q,\omega)\,S_T(0,\omega)\,]\,. \quad (1)$$

Here R_{n0} is a correction factor for the variation of the leptonic wave function over the nucleus, q is the magnitude of the three-momentum transfer, and ω the energy transfer to the nucleus. The kernel for longitudinal virtual excitations is given by

$$K_L(q,\omega) = \frac{1}{2E_q}\left[\frac{1}{(E_q-m)(\omega+E_q-m)} - \frac{1}{(E_q+m)(\omega+E_q+m)}\right] \quad (2)$$

and for transverse excitations by

$$K_T(q,\omega) = -\frac{1}{4mq}\frac{\omega+2q}{(\omega+q)^2} + \frac{q^2}{4m^2}K_L(q,\omega)\,, \quad (3)$$

where m is the mass of the lepton and fully relativistic kinematics has been retained ($E_q = \sqrt{q^2+m^2}$). This is particularly important for the electron case as the typical excitation energy of the deuteron is several MeV and the mass of the electron is only half a MeV. Finally the sea gull term has been expressed by the transverse structure function at zero momentum transfer and its kernel is given by

$$K_S(q,\omega) = \frac{1}{4m\omega}\left(\frac{1}{q} - \frac{1}{E_q}\right) . \quad (4)$$

This ensures the correct gauge condition for the two-photon amplitude, cancels the small q singularity of the transverse contribution, and should be also valid for finite q unless velocity-dependent interactions or meson exchange corrections are important.

It is convenient to write the nuclear polarization shift as

$$\Delta\epsilon_{n0} = \frac{R_{n0}}{n^3}\,\Delta\bar{\epsilon}\,, \quad (5)$$

where the shift $\Delta\bar{\epsilon}$ is independent of the atomic state. In first order of the ratio nuclear radius divided by the Bohr radius a_B the correction factor

$$R_{n0} \simeq R = 1 - 3.06\frac{\langle r^2\rangle^{1/2}}{a_B} \quad (6)$$

also turns out to be independent of the principle quantum number [10].

For the calculation of the deuteron structure functions a multipole decomposition of the usual nonrelativistic one-body charge and current operators is performed. All multipoles are taken into account, but the correct final state for the various NN potential models is considered for multipole transitions up to $L = 6$ only. The multipoles with $L > 6$, where effects of the final state interaction are negligibly small, are calculated in the plane wave Born approximation [13]. We neglect the neutron electric form factor and take for the remaining nucleon form factors the dipole fit with a dipole parameter of 0.71 GeV^2. Further details of the deuteron calculation can also be found in Ref. [14]. The double integral of the weighted structure functions in Eq. (1) is evaluated with a 72×72 Gauss integration as in Ref. [10].

Table I gives the numerical results for $\Delta\bar{\epsilon}$ when only the dominant longitudinal excitations are taken into account. For the Paris potential we also have calculated the shifts obtained with dipole excitations only: They amount to 98.9% and 91.4% of the total values for electronic and muonic deuterium, respectively. Another test calculation was the longitudinal nuclear shift for electronic deuterium with the same square well potential as used in Ref. [15]. We have obtained −18.98 kHz with our method which explicitly sums over the excited virtual states. This should be compared with the value −19.45 kHz obtained in Eq. (39) of Ref. [15] by using the long-wavelength (unretarded dipole) approximation.

TABLE I. Longitudinal reduced nuclear polarization shift $\Delta\bar{\epsilon}$ [see Eq. (5)] for electronic (e) and muonic (μ) deuterium calculated with different NN potentials. The fourth column gives the electric dipole polarizability α_{E1} of the deuteron for these potentials.

Potential	$\Delta\bar{\epsilon}^{(e)}$ [kHz]	$\Delta\bar{\epsilon}^{(\mu)}$ [meV]	α_{E1} [fm^3]
Bonn	−18.95	−12.18	0.634
Paris	−18.99	−12.20	0.635
AV14	−19.18	−12.23	0.642
Nijmegen	−19.32	−12.41	0.646

TABLE II. Transverse nuclear polarization shift for the different NN potentials. The notation is as in Table I. The values include the convection current, the spin-current, and the sea gull contribution from Eq. (1).

Potential	$\Delta\bar{\epsilon}^{(e)}$ [kHz]	$\Delta\bar{\epsilon}^{(\mu)}$ [meV]
Bonn	−2.35	−0.059
Paris	−2.36	−0.059
AV14	−2.38	−0.060
Nijmegen	−2.40	−0.060

For electronic deuterium Table II shows that the contribution of the transverse excitations is larger than the spread in the longitudinal shift generated by the different potentials. Here the convection current, the spin current, and the sea gull contributions have been taken together. For the case of the Paris potential we also checked the importance of meson exchange currents on $S_T(q,\omega)$. However, their effect is quite small, leading to a reduction of 1.3% of the corresponding value in Table II.

The total nuclear polarization shift is taken as an average over the four realistic potential models. Evaluating the correction factor from Eq. (6) we obtain $R^{(e)} = 0.9999$ and

$$\Delta\epsilon_{n0}^{(e)} = (-21.5 \pm 0.3)\ \frac{1}{n^3}\ \text{kHz}, \quad (7)$$

and with $R^{(\mu)} = 0.9778$ we get

$$\Delta\epsilon_{n0}^{(\mu)} = (-12.0 \pm 0.2)\ \frac{1}{n^3}\ \text{meV}, \quad (8)$$

where the errors reflect the spread in the values from the different potentials. This amounts to a model dependence of less than 2%.

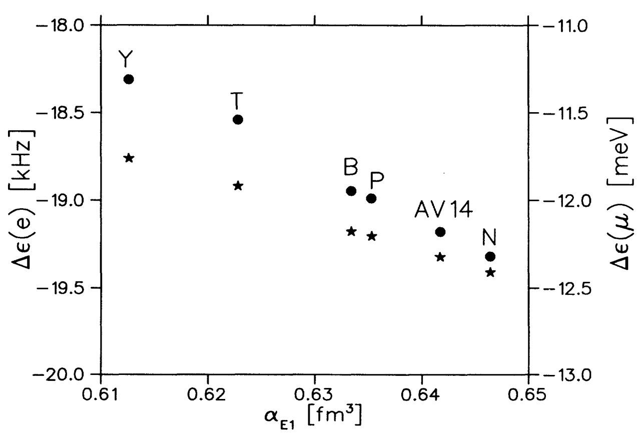

FIG. 1. Longitudinal polarization shift $\Delta\bar{\epsilon}$ as a function of the electric dipole polarizability α_{E1} for different potentials. The abbreviations denote the Yamaguchi (Y), Tabakin (T), Bonn (B), Paris (P), Argonne (AV14), and Nijmegen (N) potential. Electronic shifts are marked by dots and refer to the left axis; muonic ones are marked by stars and their values should be read off from the right axis.

Compared to the results obtained in Ref. [10] with separable potentials the present values for the nuclear polarization shift with realistic potentials are approximately 4–5 % larger in magnitude but still in the error estimate given in that paper. The discrepancy can be traced back to the different values of the electric dipole polarizability of the deuteron obtained with the different potentials which are also shown in Table I. Whereas the Yamaguchi separable potential leads to a value of 0.613 fm^3 the realistic potentials all give a higher dipole polarizability. Experimental values are in the range of 0.6–0.7 fm^3 [16]. Indeed we observe an almost *linear* dependence of our numerical results on the value of the electric dipole polarizability α_E of the deuteron produced by the specific nuclear interaction. This can be seen in Fig. 1 for the longitudinal shift where also the results from the previous semirealistic potential models are included.

The linear dependence can be qualitatively understood by invoking the unretarded dipole approximation. It is well known that in the limit $q \to 0$ the longitudinal structure function can be expressed by the total photoabsorption cross section $\sigma_\gamma(\omega)$,

$$S_L(q,\omega) \overset{q\to 0}{\longrightarrow} \frac{q^2}{4\pi^2\alpha}\,\frac{1}{\omega}\,\sigma_\gamma(\omega)\,. \tag{9}$$

The q integration in Eq. (1) can then be performed analytically with the result

$$\int_0^\infty dq\, q^2\, K_L(q,\omega) \simeq \begin{cases} \frac{\pi}{2\sqrt{2}}\sqrt{\frac{m}{\omega}} & \text{for } \omega \ll m, \\ \frac{m}{\omega}\left[\ln\left(2\frac{\omega}{m}\right)+1\right] & \text{for } \omega \gg m\,. \end{cases} \tag{10}$$

This means that in the unretarded dipole approximation the nuclear polarization shift is given by a weighted integral over the photoabsorption cross section. In agreement with well-known results in the literature Eqs. (9) and (10) determine these weights as $\omega^{-3/2}$ in the nonrelativistic (muon) case [17] and $\ln(2\omega/m)/\omega^2$ in the extreme relativistic (electron) case [18]. If, furthermore, the closure approximation is applied, the nuclear polarization shift is proportional to the dipole polarizability

$$\alpha_{E1} = \frac{1}{2\pi^2}\int_0^\infty d\omega\, \frac{1}{\omega^2}\sigma_\gamma(\omega) \tag{11}$$

multiplied by functions of the average excitation energy $\bar{E}$. These functions vary slowly as $\sqrt{\bar{E}}$ and $\ln\bar{E}$ in the nonrelativistic and in the extreme relativistic cases, respectively, so that the different mean excitation energies from the different interactions have little influence on the shift. Figure 1 shows that the linear relation between shift and dipole polarizability is indeed fulfilled to a remarkable degree of accuracy. However, as we have demonstrated for the case of the square well potential the proportionality constant in this linear relation cannot be obtained precisely with the long-wavelength or the closure approximation.

In summary, we have calculated the nuclear polarization shift in electronic and muonic deuterium with wave functions from realistic NN potentials and reduced the nuclear uncertainty considerably. This will be important for the precise analysis of future high-precision experiments in this system.

Note added. After submission of this work we were informed about two other recent calculations of the polarization shift in electronic deuterium. For the magnitude of the $1S$-$2S$ shift Martorell *et al.* obtain 19.3(2) kHz [19] and Pachucki *et al.* obtain 19(2) kHz [20] whereas our result from multiplying Eq. (7) by 7/8 is 18.8(3) kHz. Although these numbers are all consistent within the quoted errors, our value is lower mainly because we do not use the unretarded dipole approximation. We have checked numerically for the Paris potential that such an approximation leads for the longitudinal shift to an *overestimation* of the dipole contribution by about 2.5%. Omitting, furthermore, all other Coulomb multipoles and neglecting the nucleon form factor we essentially get agreement with the numbers of Refs. [19] and [20].

For the polarization shift in muonic deuterium a previous calculation [21] has obtained −9.9 meV. Although the Malfliet-Tjon potential which was employed cannot be considered as realistic, the difference from our result in Eq. (8) is much too large and deserves further investigation. We emphasize, however, that our muonic shift was obtained by the same program which was employed for calculating the electronic shift and includes all multipoles and the transverse interaction. Therefore we are confident that our result gives a realistic number for the $d\mu$ polarization shift which, incidentally, is also of some interest for muon-catalyzed fusion.

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