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Nuclear polarizabilities and logarithmic sum rules

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(Received 14 January 1997)

The electric polarizability and logarithmic mean-excitation energy are calculated for the deuteron using techniques introduced in atomic physics. These results are then used to improve limits on the atomic-deuterium frequency shift due to nuclear polarization in the unretarded dipole limit, as well as confirming previous results. [S0556-2813(97)03906-X]

PACS number(s): 21.45.+v, 13.75.Cs, 24.70.+s, 31.30.Gs

The remarkable experiments [1,2] currently being performed on the isotope shift in atomic hydrogen (^{2}H vs ^{1}H) are primarily determined by differences in the masses of the isotopes, but are significantly sensitive to nuclear structure. These measurements provide the most precise determination of the difference in sizes of these isotopes. The most recent [2] result for the d-p isotope shift in the $1S$-$2S$ level splitting is

$$\Delta\nu_{D-H}=670\,994\,334(2)\ \text{kHz}, \tag{1}$$

of which roughly 5000 kHz is attributable to the finite-size differences of the nuclei, while roughly 20 kHz is due to the electric polarizability of the deuteron. In other words, in addition to a weaker Coulomb potential arising from the nuclear charge distribution seen by the electron at very short (on the atomic scale) distances, that electron also ''distorts'' or polarizes the nucleus, which enhances the binding. Three numerical calculations of the effect of nuclear polarization on the isotope shift have been performed recently [3–5], although the relevant leading-order analytic results for the nth S state have long been known [6,7]:

$$\Delta E_{\rm pol}=-5m_e\alpha|\phi_n(0)|^2\alpha_E\left[\frac{19}{30}+\ln\left(\frac{2\overline{E}}{m_e}\right)\right], \tag{2}$$

where [8] α is the fine-structure constant, m_e is the electron mass, $|\phi_n(0)|^2=\mu^3\alpha^3/\pi n^3$ is the square of the wave function of the electron at the origin, α_E is the deuteron electric polarizability, μ is the $e-d$ reduced mass, and we work in natural units ($\hbar=c=1$). Even though uncertainties in the polarization calculations are currently smaller than the error quoted in Eq. (1), planned improvements [2] in that accuracy warrant a strong effort to reduce the theoretical uncertainty to a minimum.

The electric polarizability of a nucleus (or atom) is defined by [9]

$$\alpha_E=\frac{2\alpha}{3}\sum_{N\neq0}\frac{|\langle N|\vec{D}|0\rangle|^2}{E_N-E_0}, \tag{3}$$

where E_0 is the energy of the ground state $|0\rangle$, E_N is the energy of the Nth excited state, and $\vec{D}$ is the electric-dipole operator, which effects the transition between those states. The definition (3) can be rearranged into the form of a sum rule [9,10]:

$$\alpha_E=\frac{1}{2\pi^2}\int d\omega\,\frac{\sigma_\gamma^{\rm ud}(\omega)}{\omega^2}\equiv\frac{\sigma_{-2}}{2\pi^2}, \tag{4}$$

where $\sigma_\gamma^{\rm ud}(\omega)$ is the cross section for photoabsorption of unretarded-dipole (long-wavelength) photons by the nucleus. Concomitantly, the logarithmic mean-excitation energy in Eq. (2), $\overline{E}$, is defined by

$$\frac{2\alpha}{3}\sum_{N\neq0}\frac{|\langle N|\vec{D}|0\rangle|^2}{E_N-E_0}\ln[(E_N-E_0)/m_e]\equiv\alpha_E\ln(\overline{E}/m_e), \tag{5}$$

and clearly corresponds to placing a factor of $\ln(\omega)$ in the integrand in Eq. (4). The august σ_{-2} sum rule and its (less well-known [11]) logarithmic relative σ'_{-2} have been used to evaluate α_E and $\overline{E}$ by explicitly constructing $\langle N|\vec{D}|0\rangle$ [or equivalently, $\sigma_\gamma^{\rm ud}(\omega)$] and performing the integral numerically. Results for α_E for many ''realistic'' potential models are known, although the two most recent calculations [4,5] did not have any models in common.

In this work we will (1) calculate α_E for a set of models that subsumes most of those of Refs. [4,5] and includes several more; (2) calculate $\ln(\overline{E})$ for these models; (3) use novel (for nuclear, but not atomic, applications) numerical techniques for calculating both α_E and $\ln(\overline{E})$; (4) critically discuss the potential models and attempt to assign a subjective but credible uncertainty to the results. In this way we will confirm the previous results, while shrinking the uncertainty

associated with them. Our numerical techniques were first applied to atomic problems, but now find a comfortable home in nuclear physics.

The technique we use for calculating α_E was first used by Podolsky [12] to treat dispersion in hydrogen atoms. Definition (3) is fully equivalent to

$$\alpha_E = 2\alpha\langle 0|D_z|\Delta\Psi_z\rangle, \tag{6}$$

where

$$(H-E_0)|\Delta\Psi_z\rangle = D_z|0\rangle \tag{7}$$

is solved subject to finite boundary conditions. Note that $\vec{D}$ does not connect the ground state (the only bound state) of the deuteron to itself. Resolution of Eq. (7) into partial waves, incorporation of the nuclear (including tensor) force, and other minor (although tedious and important) details are contained in Ref. [9], together with many analytic results for simple potentials. Our calculation will employ the usual nonrelativistic (classical) dipole operator.

The resulting procedure is only slightly more complex than solving for the deuteron ground state, and it is very stable. We have calculated α_E for 14 different ''realistic'' nucleon-nucleon (NN) potential models. Such models must contain OPEP (one-pion-exchange potential), which dominates the binding of light nuclei, and they must fit the NN data reasonably well. All of the models used in Refs. [4,5] are in this category, although the quality of the fits (of various potential parameters) to the data differs rather dramatically from case to case. Most of those models could be characterized as ''first-generation'' models. Recently, the Nijmegen group and their collaborators [13–15] have constructed ''second-generation'' models, which provide good to very good quality fits to all NN data, even approaching χ^2 per degree of freedom ~ 1. Such fits are sufficiently good that they can be regarded as alternative phase-shift analyses. This does not necessarily imply that the underlying physics has a corresponding accuracy, since several of these models are purely phenomenological, except for the all-important and dominant OPEP that incorporates different pion masses in different (isospin) states.

We determine the logarithmic mean-excitation energy $\overline{E}$ (or logarithmic sum rule) using a trick developed for calculating various logarithmic mean-excitation energies in atoms [16], one of which is the Bethe logarithm. If we add a parameter $\lambda \equiv \xi \cdot f$ to $(H-E_0)$ in Eq. (7), where ξ is dimensionless and f has the dimensions of energy, we can then define (and easily calculate)

$$\alpha_E(\xi) = \frac{2\alpha}{3}\sum_{N\neq 0}\frac{|\langle N|\vec{D}|0\rangle|^2}{\xi f + E_N - E_0}, \tag{8}$$

where $\alpha_E(0)$ is the usual result. The integral of $\alpha_E(\xi)$ from 0 to Λ (very large compared to $\overline{E}/f$) generates

$$\int_0^\Lambda d\xi\,\alpha_E(\xi) \propto -\sum_{N\neq 0}\frac{|\langle N|\vec{D}|0\rangle|^2}{f}\ln[(E_N-E_0)/\Lambda f], \tag{9}$$

which gives the desired logarithm. A similar integration gives

TABLE I. Deuteron electric polarizabilities, α_E, in units of fm^3, logarithmic mean-excitation-energy ratios, $\ln(2\overline{E}/m_e)$, and deuteron $1S$-$2S$ polarization-energy shifts, $\nu_{\rm pol}$, in kHz.

Potential model	α_E (fm^3)	$\ln(2\overline{E}/m_e)$	$\nu_{\rm pol}$(kHz)
Second-generation potentials			
Reid Soft Core (93)	0.6345	2.9616	19.31
Argonne V_{18}	0.6343	2.9625	19.31
Nijmegen (loc-rel)	0.6334	2.9618	19.28
Nijmegen (loc-nr)	0.6327	2.9624	19.26
Nijmegen (nl-rel)	0.6328	2.9619	19.26
Nijmegen (nl-nr)	0.6319	2.9625	19.24
Nijmegen (full-rel)	0.6311	2.9615	19.21
First-generation potentials			
Reid Soft Core (68)	0.6237	2.9638	18.99
Bonn (CS)	0.6336	2.9630	19.29
Paris	0.6352	2.9627	19.34
de Tourreil–Rouben–Sprung	0.6376	2.9623	19.41
Argonne V_{14}	0.6419	2.9624	19.54
Nijmegen (78)	0.6472	2.9612	19.70
Super Soft Core (C)	0.6497	2.9617	19.77

$$\int_\epsilon^\infty \frac{d\xi}{\xi}\alpha_E(\xi) \propto \sum_{N\neq 0}\frac{|\langle N|\vec{D}|0\rangle|^2}{E_N-E_0}\ln[(E_N-E_0)/\epsilon f]. \tag{10}$$

For numerical purposes, we split the integral in Eq. (10) into $\int_\epsilon^1 + \int_1^\infty$, and the dimensionful scale parameter f determines where the split occurs in energy units. Rearranging slightly and changing variables to $1/\xi$ in the second integral, we achieve our final result:

$$\alpha_E(0)\ln(2\overline{E}/m_e) = \int_0^1 \frac{d\xi}{\xi}[\alpha_E(\xi)-\alpha_E(0)+\alpha_E(1/\xi)] - \alpha_E(0)\ln(m_e/2f). \tag{11}$$

The integrand is finite everywhere. Choosing $f \sim 3-5|E_0|$ makes the integral converge to five significant figures with only a few (~ 6) Gauss-quadrature points, and all results for $\overline{E}$ are independent of f if the integrals are performed with sufficient accuracy. Podolsky's method [9,12] makes the calculation of $\alpha_E(\xi)$ as easy as that of $\alpha_E(0)$. The method is very stable.

Table I presents our results for α_E, $\ln(2\overline{E}/m_e)$, and $\Delta E_{\rm pol}$ separated into first-generation [17–23] (listed in order of appearance in Table I) and second-generation [13–15] (potential) categories. Note that there is much more spread in the first-generation results, reflecting indifferent fits to the NN data. The spread in the second-generation results can be summarized by

$$\nu_{\rm pol} = 19.26(6)\ \text{kHz} \tag{12}$$

and

$$\alpha_E = 0.6328(17)\ \text{fm}^3. \tag{13}$$

As noted below in Ref. [4], this is not a numerically complete result for the sum of all polarizability corrections, since

it incorporates only unretarded dipole approximation. Higher multipoles, retarded dipole contributions, seagulls, etc., have not been included here, and may decrease this result by up to 1 kHz [4].

All of the appropriate results are quite close to those previously calculated [4,5], with the electric polarizabilities differing at most by 2 in the last quoted significant figure in those references. Such small differences could be attributed to slightly different versions of the potentials (new potentials are often a matter of ''work in progress''). Note also that the pairs of new Nijmegen [14] local and nonlocal potentials (labeled ''loc'' and ''nl'' in Table I) have versions with relativistic (''rel'') and nonrelativistic (''nr'') kinematics (corresponding to *identical* deuteron energies of $2\sqrt{M^2-\kappa_{\rm rel}^2}-2M$ or $-\kappa_{\rm nr}^2/M$, respectively). The slightly smaller value of $\kappa_{\rm rel}$ in the (excellent) zero-range approximation [5,9] accounts for those differences in the values of α_E, although this makes relatively little difference in $\nu_{\rm pol}$. The ''full'' Nijmegen potential [14] has the same form in all partial waves and fits the *NN* data less well than the others.

The result (13) agrees very well with a prediction [9] of $\alpha_E = 0.632(3)\ \text{fm}^3$ made many years ago, and this warrants further comment. One can perform perturbation theory about the ''zero-range'' limit by turning off the forces in *p* waves, dropping the deuteron *d* state, and replacing the (reduced) deuteron *s*-state wave function by its asymptotic form: $u(r)=A_S\exp(-\kappa r)$, where A_S is the *s* wave asymptotic normalization constant. With this ansatz we obtain [5,9]

$$\alpha_E \cong \alpha_E^0 = \frac{\alpha\mu A_S^2}{32\kappa^5}, \tag{14}$$

where here μ is the *n*-*p* reduced mass, and $\ln(2\overline{E}/m_e)=2.9671$. This remarkably simple formula overestimates the complete result by approximately 1%. There is little uncertainty in any of the quantities except for A_S, which was recently determined [24] to be $A_S = 0.8845(8)\ \text{fm}^{-1/2}$ in agreement with the value used in Ref. [9], and which leads to $\alpha_E^0 = 0.6378(12)\ \text{fm}^3$. Moreover, the corrections, $\Delta\alpha_E$, to α_E^0 defined by $\alpha_E=\alpha_E^0+\Delta\alpha_E$ can be determined from the potential models (see Refs. [5,9]) to be $\Delta\alpha_E\cong -0.0044(2)\ \text{fm}^3$, which leads directly to $\alpha_E=0.6334(14)\ \text{fm}^3$, which is consistent with Eq. (13). Note that no relativistic corrections have been incorporated and they are not likely to be negligible on the scale of the uncertainty in Eq. (13).

Why do the ''second-generation'' potentials agree so well with the perturbation theory estimates? The answer is that A_S is determined by analyzing *NN* scattering, and we stated earlier that the new potentials could be viewed as alternative phase-shift analyses. That is, they fit the *NN* data quite well, and associated properties (such as A_S) should agree with other experimental determinations. Thus, α_E is very well determined.

We summarize by noting that α_E and $\ln(\overline{E})$ have been calculated for the deuteron by novel methods. These calculations confirm previous results and add additional ones. We strongly recommend that only second-generation potential results be used when assessing the reliability of α_E calculations. Equation (12) gives our best estimate for the leading-order (unretarded-dipole or long-wavelength) approximation to the nuclear-polarizability correction given by Eq. (2).

Note added in proof. S. Karshenboim informed us that we overlooked the zero-range calculations in A. I. Milshtein, I. B. Khriplovitch, and S. S. Petrosyan, Zk. Eksp. Teor. Fiz. **109**, 1146 (1996) [Sov. Phys. JETP **82**, 616 (1996)]. We thank Dr. Karshenboim.

The work of J.L.F. was performed under the auspices of the U.S. Department of Energy, while that of G.L.P. was supported in part by the U.S. Department of Energy. One of us (J.L.F.) would like to thank Don Sprung and Winfried Leidemann for helpful discussions of their results.

[1] K. Pachucki, D. Leibfried, M. Weitz, A. Huber, W. Konig, and T. W. Hänsch, J. Phys. B **29**, 177 (1996) is an excellent review of recent experimental and theoretical progress.

[2] T. W. Hänsch (unpublished); efforts are under way to reduce this uncertainty by an order of magnitude, T. W. Hänsch (private communication).

[3] K. Pachucki, D. Leibfried, and T. W. Hänsch, Phys. Rev. A **48**, R1 (1993); K. Pachucki, M. Weitz, and T. W. Hänsch, *ibid.* **49**, 2255 (1994).

[4] W. Leidemann and R. Rosenfelder, Phys. Rev. C **51**, 427 (1995); Y. Lu and R. Rosenfelder, Phys. Lett. B **319**, 7 (1993). This work goes beyond our Eq. (2), and includes retardation and higher multipoles.

[5] J. Martorell, D. W. L. Sprung, and D. C. Zheng, Phys. Rev. C **51**, 1127 (1995). The individual results of this paper differ from ours by 0.07 kHz, because their unretarded dipole approximation contains additional small terms from the electron kinematics.

[6] J. Bernabéu and T. E. O. Ericson, Z. Phys. A **309**, 213 (1983).

[7] J. L. Friar (unpublished); reference [6] appeared just before the completion of this work, which was an extension of Ref. [11] from muonic to electronic atoms. This work nevertheless used completely different techniques (Euclidean four-dimensional spherical coordinates) to perform the integrals and verified the results of Ref. [6].

[8] E. R. Cohen and B. N. Taylor, Rev. Mod. Phys. **59**, 1121 (1987). All constants are taken from this work.

[9] J. L. Friar and S. Fallieros, Phys. Rev. C **29**, 232 (1984).

[10] J. L. Friar, S. Fallieros, E. L. Tomusiak, D. Skopik, and E. G. Fuller, Phys. Rev. C **27**, 1364 (1983). This reference uses Eq. (4) to obtain $\alpha_E=0.61(4)\text{fm}^3$; see also N. L. Rodning, L. D. Knutson, W. G. Lynch, and M. B. Tsang, Phys. Rev. Lett. **49**, 909 (1982), which obtained $\alpha_E=0.70(5)\text{fm}^3$.

[11] J. L. Friar, Phys. Rev. C **16**, 1540 (1977).

[12] B. Podolsky, Proc. Natl. Acad. Sci. USA **14**, 253 (1928).

[13] J. L. Friar, G. L. Payne, V. G. J. Stoks, and J. J. de Swart, Phys. Lett. B **311**, 4 (1993).

[14] V. G. J. Stoks, R. A. M. Klomp, C. P. F. Terheggen, and J. J. de Swart, Phys. Rev. C **49**, 2950 (1994).

[15] R. B. Wiringa, V. G. J. Stoks, and R. Schiavilla, Phys. Rev. C

51, 38 (1995).
[16] S. Rosendorff and A. Birman, Phys. Rev. A **31**, 612 (1985).
[17] R. V. Reid, Ann. Phys. (N.Y.) **50**, 411 (1968).
[18] R. Machleidt, K. Holinde, and C. Elster, Phys. Rep. **149**, 1 (1987).
[19] M. LaCombe *et al.*, Phys. Rev. C **21**, 861 (1980).
[20] R. de Tourreil, B. Rouben, and D. W. L. Sprung, Nucl. Phys. **A242**, 445 (1975).
[21] R. B. Wiringa, R. A. Smith, and T. A. Ainsworth, Phys. Rev. C **29**, 1207 (1984).
[22] M. M. Nagels, T. A. Rijken, and J. J. de Swart, Phys. Rev. D **17**, 768 (1978).
[23] R. de Tourreil and D. W. L. Sprung, Nucl. Phys. **A201**, 193 (1973).
[24] J. J. de Swart, C. P. F. Terheggen, and V. G. J. Stoks, *Proceedings of the Third International Symposium Dubna Deuteron 95*, Dubna, Russia, 1995 (Nijmegen Report THEF-NYM-95.11, nucl-th/9509032, 1995); J. J. de Swart, R. A. M. Klomp, M. C. M. Rentmeester, and Th. A. Rijken, Few-Body Syst. Suppl. **99**, (1995).