Electric Polarization of the Deuteron by a Point Charge*

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The perturbation of the ground-state energy of the deuteron due to a fixed point charge at any distance is calculated, using the method of Dalgarno and Lewis and a simple ground-state wave function. Deviations from the uniform field results are evaluated for various distances and amount to about 5% for regions of interest.

I. INTRODUCTION

THE effect on the deuteron of an external, uniform electric field has been calculated in various approximations by several authors.[1] Recently, Clement[2] has re-examined this problem, and has considered its application to deuteron scattering from light nuclei.

In particular, Clement[2] has used the adiabatic approximation for the center-of-mass motion; that is, the internal motion of the nucleons in the deuteron is assumed to be rapid compared to the motion of the deuteron itself. Under these conditions, the electric field of the scatterer polarizes the deuteron, and the perturbation in the energy produced by the field is treated as an addition to the scattering potential, which depends only on the distance between the deuteron and the scatterer.

For large impact-parameter scattering, the field is nearly uniform, and its magnitude follows an inverse square law. In second-order perturbation theory, the adiabatic polarization potential thus obeys an inverse fourth-power law asymptotically. For closer collisions this potential cannot be used since it gives divergent results and must be cut off at a reasonably large radius. In addition, as the collision distance diminishes, higher multipole terms in the electric field enter.

In the present paper, a simple wave function is used for the unperturbed deuteron, and the adiabatic polarization potential is calculated using the method of Dalgarno and Lewis[3] to carry out the second-order perturbation sums. General results are obtained for any multipole and for all distances. In particular, the short-range modifications to the leading (dipole) part are exhibited explicitly, and long-range contributions are evaluated for all multipoles and are rewritten in terms of a single integral. A discussion of the experimental relevance of the theory is also given.

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II. CALCULATION OF THE POLARIZATION ENERGY

The Hamiltonian for a deuteron in the field of a point charge Ze fixed at the origin is

$$H=-\frac{\hbar^2}{2M}[\nabla_p^2+\nabla_n^2]+V(\mathbf{r}_p-\mathbf{r}_n)+\frac{Ze^2}{r_p}. \tag{1}$$

The definitions of the symbols are self-evident, the internucleon potential will be treated as central, and the neutron-proton mass difference is neglected. A standard transformation to center-of-mass coordinate $\mathbf{x}=\frac{1}{2}(\mathbf{r}_p+\mathbf{r}_n)$ and relative coordinate $\mathbf{r}=\mathbf{r}_n-\mathbf{r}_p$ puts the Hamiltonian into the form

$$H=-\frac{\hbar^2}{4M}\nabla_x^2-\frac{\hbar^2}{M}\nabla_r^2+V(r)+\frac{Ze^2}{|\mathbf{x}-\frac{1}{2}\mathbf{r}|}. \tag{2}$$

The adiabatic (or Born-Oppenheimer) approximation treats $\mathbf{x}$ as a parameter at first, evaluates the energy of the internal motion as a function of $\mathbf{x}$, and then uses this energy as the potential in a second Schrödinger equation for the center-of-mass motion.

Specifically, one considers two unperturbed Hamiltonians

$$H_{0x}=-\frac{\hbar^2}{4M}\nabla_x^2+\frac{Ze^2}{x} \tag{3a}$$

and

$$H_{0r}=-(\hbar^2/M)\nabla_r^2+V(r), \tag{3b}$$

plus the perturbation

$$H'=Ze^2\left[\frac{1}{|\mathbf{x}-\frac{1}{2}\mathbf{r}|}-\frac{1}{x}\right]. \tag{3c}$$

The plan is then to calculate the change in the eigenvalue of H_{0r} induced by H' up to second order, which yields what can be called the adiabatic perturbing potential $V(x)$ that modifies the pure Coulomb scattering given by H_{0x}.

The first-order calculation is simple, and only yields short-range contributions. If $\Phi(r)$ is the unperturbed, normalized deuteron ground-state wave function, one obtains

$$V_1(x)=\int d^3r\,|\Phi(r)|^2H'$$
$$=4\pi e^2Z\int_{2x}^{\infty}dr\,r^2|\Phi(r)|^2\left[\frac{2}{r}-\frac{1}{x}\right]. \tag{4}$$

Since $\Phi(r)$ is appreciable only out to the deuteron "radius," and $r>2x$ in the above integral, the potential $V_1(x)$ is short-ranged. It will be evaluated later for a specific form of wave function.

The second-order adiabatic potential is

$$V_2(x)=\sum_{n\neq 0}\frac{\langle 0|H'|n\rangle\langle n|H'|0\rangle}{E_0-E_n}, \tag{5}$$

where the states $|0\rangle$ and $|n\rangle$ are the ground and excited states of the deuteron system. To carry out the summation over the excited intermediate states, the method of Dalgarno and Lewis,[3] recently extensively discussed and applied by Schwartz,[4] will be employed. In this method one must solve the equation

$$[F,H_{0r}]|0\rangle=[H'-\langle 0|H'|0\rangle]|0\rangle \tag{6}$$

for the function F, where $|0\rangle$ is the known ground-state vector of H_{0r}. Then the second-order adiabatic potential is

$$V_2(x)=\langle 0|H'F|0\rangle-\langle 0|H'|0\rangle\langle 0|F|0\rangle, \tag{7}$$

after the completeness relation

$$\sum_{n\neq 0}|n\rangle\langle n|=1-|0\rangle\langle 0|$$

has been invoked. Note that $\langle 0|H'|0\rangle\equiv V_1(x)$.

Equation (6) can be solved analytically only for quite simple or special ground-state functions. One of these is the zero-range central wave function for the deuteron,

$$\Phi(r)=\left(\frac{\gamma}{2\pi}\right)^{1/2}\frac{e^{-\gamma r}}{r}, \tag{8}$$

where $\hbar^2\gamma^2M^{-1}=E_B$, the deuteron binding energy. This satisfies the Schrödinger equation outside the range of the potential only, and cannot be trusted for small r. Next, the perturbing Hamiltonian is expanded in the usual Legendre polynomial series, both for $r<2x$ and $r>2x$:

$$H'=\sum_{l=0}^{\infty}\mathcal{H}_l(x,r)P_l(\cos\theta), \tag{9}$$

$$\mathcal{H}_{l<}(x,r)=\frac{Ze^2}{x}\left[\left(\frac{r}{2x}\right)^l-\delta_{l0}\right] \quad \text{for} \quad r<2x, \tag{9a}$$

$$\mathcal{H}_{l<}(x,r)=\frac{Ze^2}{x}\left[\left(\frac{2x}{r}\right)^{l+1}-\delta_{l0}\right] \quad \text{for} \quad r>2x, \tag{9b}$$

where the notation is self-explanatory. With this expansion, and the similar one for the function F,

$$F(\mathbf{x},\mathbf{r})=\sum_{l=0}^{\infty}F_l(x,r)P_l(\cos\theta), \tag{10}$$

it is easily shown that Eq. (6) becomes

$$\frac{d^2F_l}{dr^2}-2\gamma\frac{dF_l}{dr}-\frac{l(l+1)}{r^2}F_l=Q_l, \tag{11}$$

where

$$Q_l=\frac{M}{\hbar^2}[\mathcal{H}_l-V_1(x)\delta_{l0}], \tag{11a}$$

and the function $\Phi(r)$ in Eq. (8) is used and assumed to be an eigenfunction of H_{0r}.

Particular solutions $\bar{F}_l$ of Eq. (11) can be easily obtained for $l\neq 0$ for both inside and outside regions in r:

$$\bar{F}_{l<}(x,r)=-\frac{ZMe^2}{\hbar^2\gamma(l+1)}\left(\frac{r}{2x}\right)^{l+1}, \tag{12a}$$

$$\bar{F}_{l>}(x,r)=\frac{ZMe^2}{\hbar^2\gamma l}\left(\frac{2x}{r}\right)^{l}. \tag{12b}$$

These functions are well behaved at $r=0$ and $r\to\infty$, and, surprisingly, their first derivatives with respect to r are continuous everywhere, including $r=2x$. The functions themselves, however, do not join continuously at $r=2x$. Therefore, the general solution of the homogeneous equation obtained from Eq. (11) must be considered. This equation is of a type which yields Bessel's equation upon appropriate substitutions. The complete solutions, properly behaved at the boundary points and properly continuous at $r=2x$, can be found with some effort to be [for $l\neq 0$]

$$F_{l<}(x,r)=-\frac{ZMe^2}{\hbar^2\gamma(l+1)}\times\left[\left(\frac{r}{2x}\right)^{l+1}-\left(\frac{2l+1}{l}\right)\gamma r e^{\gamma(r-2x)}j_l(i\gamma r)\bar{h}_l\right], \tag{13a}$$

$$F_{l>}(x,r)=\frac{ZMe^2}{\hbar^2\gamma l}\times\left[\left(\frac{2x}{r}\right)^{l}+\left(\frac{2l+1}{l+1}\right)\gamma r e^{\gamma(r-2x)}h_l(i\gamma r)\bar{j}_l\right], \tag{13b}$$

where $j_l(z)$ is the spherical Bessel function of order l, $h_l(z)$ is the spherical Hankel function of the first kind of order l, and

$$\bar{j}_l\equiv(2\gamma x+1)j_l(2i\gamma x)+x\,dj_l(2i\gamma x)/dx, \tag{14a}$$

$$\bar{h}_l\equiv(2\gamma x+1)h_l(2i\gamma x)+x\,dh_l(2i\gamma x)/dx. \tag{14b}$$

For $l=0$, the inhomogeneous equation is of first order in dF_0/dr and can be integrated directly, while the

[4] C. Schwartz, Ann. Phys. (N. Y.) 2, 156 (1959).

homogeneous equation is trivial. The result is

$$F_{0<}(x,r)=-\frac{ZMe^2}{2\gamma\hbar^2}\left[\left(-r+\frac{e^{2\gamma r}}{2\gamma}\right)\frac{V_1(x)}{Ze^2}+2\ln(2\gamma x)-2+\frac{1}{2\gamma x}\right], \quad (15a)$$

$$F_{0>}(x,r)=-\frac{ZMe^2}{2\gamma\hbar^2}\left\{-r\left[\frac{1}{x}+\frac{V_1(x)}{Ze^2}\right]-2e^{2\gamma r}\,\mathrm{Ei}(-2\gamma r)+2\ln(\gamma r)\right\}, \quad (15b)$$

where

$$\mathrm{Ei}(-z)=-\int_z^\infty e^{-y}dy/y,$$

and the first-order potential is

$$V_1(x)=-Ze^2[x^{-1}e^{-4\gamma x}+4\gamma\,\mathrm{Ei}(-4\gamma x)]. \quad (15c)$$

To evaluate the adiabatic potential $V_2(x)$ we insert the above expressions in Eq. (7), and carry out the integrations over $\mathbf{r}$ for each term in the multipole expansion.

III. EVALUATION OF THE ADIABATIC PERTURBING POTENTIAL

In this section the dipole ($l=1$) term in $V_2(x)$ will be evaluated. This part is dominant at large distances, and its shorter range parts are also of interest.

For the dipole term one must evaluate

$$V_2^{(1)}(x)=\frac{\gamma}{2\pi}\int d^3r\,\frac{e^{-2\gamma r}}{r^2}\mathfrak{C}_1F_1[P_1(\cos\theta)]^2. \quad (16)$$

The angular integration is carried out, the convenient change of variables $t=2\gamma x$, $y=\gamma r$ is made, and one obtains

$$V_2^{(1)}(t)=\frac{2}{3}\frac{Z^2Me^4}{\hbar^2}\left\{-t^{-4}\int_0^t dy\,y^3e^{-2y}+3t^{-2}e^{-t}\bar{h}_1\int_0^t dy\,y^2e^{-y}j_1(iy)+2t^2\int_t^\infty dy\,y^{-3}e^{-2y}+\tfrac{3}{2}te^{-t}\bar{j}_1\int_t^\infty dy\,y^{-1}e^{-y}h_1(iy)\right\}, \quad (17)$$

where

$$\bar{j}_1=(1/2i)[e^t(-2+2t^{-1}-t^{-2})+e^{-t}t^{-2}],$$
$$\bar{h}_1=-it^{-2}e^{-t},$$
$$j_1(iy)=(1/2i)[e^y(y^{-2}-y^{-1})-e^{-y}(y^{-2}+y^{-1})],$$
$$h_1(iy)=ie^{-y}(y^{-2}+y^{-1}).$$

After carrying out the integrals in Eq. (17), one obtains the following explicit potential due to the $l=1$ terms:

$$V_2^{(1)}(t)=\frac{2Z^2Me^4}{3\hbar^2t^4}\times\left\{-\tfrac{3}{8}+e^{-2t}\left[-2t^5+t^4-\tfrac{1}{4}t^3+3t^2-\frac{21t}{8}+\frac{21}{8}\right]-e^{-4t}[(9t/8)+9/4]-4t^6\,\mathrm{Ei}(-2t)\right\}. \quad (18)$$

The asymptotic leading term is the t^{-4} term and agrees with Clement's[2] results for the zero-range wave function.

To examine the principal corrections to the leading term, it is convenient to use the well-known asymptotic expansion for the exponential integral[5]:

$$\mathrm{Ei}(-x)\sim-\frac{e^{-x}}{x}\sum_{n=0}^{N}\frac{n!(-1)^n}{x^n}. \quad (19)$$

Using this form in Eq. (18), one obtains the approximate result

$$V_2^{(1)}(t)\sim-\frac{Z^2Me^4}{4\hbar^2t^4}\left\{1-e^{-2t}(2t^3+4t^2+t-13)+3e^{-4t}(t+2)-\frac{16}{3}t^5e^{-2t}\sum_{n=6}^{N}\frac{n!(-1)^n}{(2t)^n}\right\}, \quad (20)$$

where the asymptotic series is terminated in the usual way. The effect is shown in Table I, where D is defined as the fractional deviation of $V_2^{(1)}(t)$ due to its departure from t^{-4} behavior, and ΔD is the uncertainty in D produced by the asymptotic expansion. The deviation is seen to be appreciable as far out as $t=4$–5 or $x=9$ F. Clement[2] has discussed the typical case of deuteron scattering from Co^{59} at 3.32 MeV, for which the principal contribution to the scattering is the region $x\approx12$ F, although the cutoff is made at the nuclear radius, $x\approx6$ F ($t\approx2.7$).

TABLE I. The deviation of the dipole polarization potential from t^{-4} form: $V_2^{(1)}(t)\sim(Z^2Me^4/4\hbar^2t^4)(1+D)$. The dimensionless parameter t is related to the deuteron center-of-mass position by $x=t/2\gamma=2.2t$ F, and ΔD is the error due to the asymptotic expansion discussed in the text.

t	D	ΔD
3	−0.223	±0.025
4	−0.065	±0.002
5	−0.016	···
6	−0.004	···

[5] E. Jahnke and F. Emde, *Tables of Functions* (Dover Publications, Inc., New York, 1945), p. 3.

One can easily examine the limit of the dipole polarization potential as $t \to 0$. This is done by expanding the exponentials in Eq. (18), and gives the result $V_2^{(1)}(0) = Z^2Me^4/2\hbar^2$. The fact that this result is positive, while second-order perturbation theory must give a negative result for all t, is due to the incorrectness of the zero-range wave function at short distances. In fact $V_2^{(1)}(t)$ is not analytic at $t=0$. Better wave functions have been discussed by Clement,[2] including the Hulthén function, but their use does not seem justified in the present context. One should simply restrict oneself to consideration of the large-t parts of the potential.

IV. SUMMATION OF THE DOMINANT LONG-RANGE TERMS

It is interesting to examine the complete series for the polarization potential[6] at very large t; that is, the part given by $\bar{F}_{l<}$ in Eq. (12a). The potential due to this asymptotic part is

$$\bar{V}(t) = \langle 0 | H_<' F_< | 0 \rangle = -\frac{4Z^2Me^4}{\hbar^2}\int_0^1 dp\, e^{-2tp} G(p), \quad (21)$$

where

$$G(p) = \sum_{l=1}^{\infty} p^{2l+1}[(l+1)(2l+1)]^{-1}, \quad p = r/2x. \quad (21a)$$

The first method of calculation consists in integrating $G(p)$ term by term, which yields the following result:

$$\bar{V}(t) = -\frac{4Z^2Me^4}{\hbar^2}\left[\sum_{l=1}^{\infty}\frac{(2l)!}{l+1}(2t)^{-2(l+1)} - e^{-2t}R(t)\right], \quad (22)$$

where $R(t)$ is a rather complicated remainder term, which is a series in $(2t)^{-1}$. Because of the exponential factor which tends to damp out the remainder term, the series shown is dominant at large t. Nevertheless it is only semiconvergent since the ratio of two successive term approaches $(l/t)^2$. In Table II the semiconvergent series is evaluated and its error estimated, and is presented as a ratio to be compared with the leading ($l=1$) term.

TABLE II. Effect of higher multipoles in the large t region. The asymptotic expansion in Eq. (22) appears as the ratio to the leading dipole term, its estimated error is given, and the exact ratio is in the last column.

t	Asymptotic ratio	Error	Exact ratio
3	1.22	0.14	1.042
4	1.17	0.03	1.098
5	1.106	0.006	1.07_8
6	1.068	0.001	1.04_6

[6] Work similar to this has been carried out, for the case of the polarizability of atomic hydrogen, by the following: A. Temkin, Phys. Rev. **116**, 358 (1959), and A. Dalgarno and N. Lynn, Proc. Phys. Soc. (London) **A70**, 223 (1957).

The second method is to compute the sum defining $G(p)$ and subsequently carry out the integration over p. One can easily show by differentiating term by term, and summing, that $G(p)$ satisfies the following equation:

$$\frac{p}{2}\frac{d^2G}{dp^2} + \frac{dG}{dp} = \frac{p^2}{1-p^2}. \quad (23)$$

This has the easily verified solution,

$$G(p) = p^{-1}[(1+p)\ln(1+p) + (1-p)\ln(1-p)] - p, \quad (24)$$

which can also be shown to give the series, Eq. (21a), for $p<1$. In Table II this latter result also appears; it contains the whole effect of $\bar{F}_{l<}$, including the remainder term, and was evaluated numerically, using the Brandeis University RPC-4000 electronic computer which was kindly programmed and operated by Professor Milton Baker.

V. CONCLUSIONS AND DISCUSSION

A simplified deuteron model has been used to illustrate the procedure for calculating the adiabatic polarization potential between a point charge and a slowly moving deuteron, for all multipoles, in second-order perturbation theory. The higher multipoles make small, but not necessarily negligible, contributions to the potential, which is dominated by the inverse fourth-power behavior due to the dipole term.

For future investigation one might include the use of better unperturbed deuteron wave functions. Although other analytical solutions of Eq. (6) probably do not exist, numerical quadrature by machine should be easy. Higher order effects in the mutual polarization of two deuterons might also be considered. Analysis of experiments other than those discussed by Clement[2] can also be attempted.

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