Variation Calculation of the Polarizability of the Deuteron

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The polarizability of the deuteron in a uniform electric field is calculated by a variation method. The result obtained by Ramsey, Malenka, and Kruse is rederived and improved in accuracy, and the modification of the deuteron wave function produced by the electric field is calculated.

In a recent paper, Ramsey, Malenka, and Kruse[1] presented an approximate calculation of the electric polarizability of the deuteron. The purpose of the present paper is to rederive their result from a variation principle and to improve the accuracy. The modification of the deuteron wave function produced by the electric field is also found.

The Schrödinger equation for the relative motion in the center-of-mass system of a deuteron in a uniform electric field is

$$(H_0+H'-E)\psi=0. \tag{1}$$

The perturbation is $H'=-\frac{1}{2}e\mathcal{E}z$; z is the component of the relative n-p separation vector along the electric field, $\mathcal{E}$. A trial function $\psi=\psi_0+\mathcal{E}\phi$ is taken; ϕ may depend on $\mathcal{E}$. ψ_0 is the normalized, even-parity ground-state wave function, which satisfies the equation:

$$(H_0-E_0)\psi_0=0. \tag{2}$$

With the assumed trial function, the lowest energy level satisfies the variational inequality:

$$E\leqq\frac{\int(\psi_0^*+\mathcal{E}\phi^*)(H_0+H')(\psi_0+\mathcal{E}\phi)d\tau}{\int(\psi_0^*+\mathcal{E}\phi^*)(\psi_0+\mathcal{E}\phi)d\tau}. \tag{3}$$

In Eq. (3) and all subsequent expressions, the appropriate spin sums are implied. With Eq. (2), Eq. (3) can be written:

$$E\leqq E_0+\mathcal{E}^2\Big\{\frac{1}{\mathcal{E}}\int\psi_0^*H'\phi d\tau+\frac{1}{\mathcal{E}}\int\phi^*H'\psi_0d\tau+\int\phi^*(H_0-E_0)\phi d\tau-E_0\Big[\int\psi_0^*\phi d\tau+\int\phi^*\psi_0d\tau\Big]^2\Big\}+O(\mathcal{E}^3). \tag{4}$$

ϕ is taken to be that function which minimizes the right-hand side (rhs) of Eq. (4). Both ψ_0 and ϕ can be considered to be three-component wave functions, each component being associated with one of the possible values of the z component of the spin.[2] The rhs of Eq. (4) can be minimized by equating to zero its variation with respect to one component of ϕ^*. This process yields a differential equation for ϕ:

$$(H_0-E_0)\phi=-\frac{1}{\mathcal{E}}H'\psi_0+2E_0\psi_0\Big\{\int\psi_0^*\phi d\tau+\int\phi^*\psi_0d\tau\Big\}+O(\mathcal{E}). \tag{5}$$

The polarizability is determined by that term of $E-E_0$ which is quadratic in $\mathcal{E}$. From Eq. (4) it is clear that only that part of ϕ which is of zero order in $\mathcal{E}$ affects the polarizability. If ϕ is expressed as the sum of an even parity function and an odd parity function, Eq. (5) shows that only the odd parity function has a term of zero order in $\mathcal{E}$.[3] If only those quantities which affect the polarizability are considered, Eq. (5) becomes

$$(H_0-E_0)\phi=-\frac{1}{\mathcal{E}}H'\psi_0=\frac{e}{2}z\psi_0. \tag{6}$$

The polarizability is $\alpha=-2(E-E_0)/\mathcal{E}^2$; with this and Eq. (6), Eq. (4) yields[4]

$$\alpha=-\frac{2}{\mathcal{E}}\int\psi_0^*H'\phi d\tau=e\int\psi_0^*z\phi d\tau. \tag{7}$$

The odd parity solution of Eq. (6) is

$$\phi=\frac{e}{2}\int G(\mathbf{r},\mathbf{r}')z'\psi_0(\mathbf{r}')d\tau'; \tag{8}$$

$G(\mathbf{r},\mathbf{r}')$ is the deuteron Green's function.[5] With Eq.

[1] Ramsey, Malenka, and Kruse, Phys. Rev. 91, 1162 (1953).

[2] The singlet spin function need not be considered, because the perturbation H' does not connect singlet and triplet spin states.

[3] If the even parity function has a zero-order term, it must be a multiple of ψ_0; this cannot affect the polarizability.

[4] As a result of the variation process, Eq. (7) is an equality. That Eq. (7) is exact can be seen from an examination of Eq. (1): If $\psi=\psi_0+\mathcal{E}\phi$ is considered to be an eigenfunction, and ϕ is expressed as the sum of an even parity function and an odd parity function, then Eq. (1) can be separated into an even parity equation and an odd parity equation. These two equations show that Eq. (7) is exact and that the zero-order term of ϕ has odd parity and satisfies Eq. (6).

[5] Equation (8) can also be derived from perturbation theory, in analogy with the derivation by Ramsey *et al.* of their Eq. (5).

(8), Eq. (7) becomes

$$\alpha=\frac{e^2}{2}\int\int\psi_0^*(\mathbf{r})zG(\mathbf{r},\mathbf{r}')z'\psi_0(\mathbf{r}')d\tau'd\tau. \quad (9)$$

Equation (9) is the expression for α obtained by Ramsey *et al.*[1] by means of the Schrödinger perturbation theory. They approximated Eq. (9) by replacing the Green's function for the deuteron with that for a free particle. From Eqs. (6) and (8), it is clear that this approximation is equivalent to the assumption that the n-p interaction vanishes for odd parity states (Serber interaction). Ramsey *et al.*[1] have shown that, with the free-particle Green's function, Eq. (9) can be separated conveniently into contributions arising from the ground-state S wave alone (α_{SS}), from the D wave alone (α_{DD}) and from cross terms involving both S and D waves (α_{SD}).

Equation (8) has been used to calculate the modification ϕ_S of the ground-state S wave in two cases: The n-p interaction V_d is taken to be (1) a Serber interaction and (2) a (scalar) square well interaction for odd-parity states. In calculations which involve only the ground-state S wave, the spin functions can be omitted; the S wave ψ_S is taken to be the Hulthén wave function:

$$\psi_S=N\{e^{-\gamma r}-e^{-(\gamma+\beta)r}\}/r, \quad (10)$$

N is so chosen that the ground state is 96 percent S state. $\gamma^2=(2\mu/\hbar^2)\epsilon$; $\epsilon=-E_0=2.226$ Mev, and μ is the reduced mass. The Hulthén range parameter β is taken to be $\beta=6.0\gamma$.

Case 1. V_d a Serber Interaction

With the free-particle Green's function $G_f(\mathbf{r},\mathbf{r}')$ and $\psi_0=\psi_S$, Eq. (8) yields

$$\phi_S^{(1)}=\frac{e\mu}{\hbar^2}N\cos\theta\left\{\frac{1}{4\gamma}re^{-\gamma r}-\frac{1}{\beta^2(2\gamma+\beta)^2}\left[\frac{2(1+\gamma r)}{r^2}e^{-\gamma r}-\frac{2}{r^2}e^{-(\gamma+\beta)r}-\frac{2(\gamma+\beta)}{r}e^{-(\gamma+\beta)r}-\beta(2\gamma+\beta)e^{-(\gamma+\beta)r}\right]\right\}. \quad (11)$$

With this $\phi_S^{(1)}$ and Eq. (7), one gets[1]

$$\alpha_{SS}^{(1)}=0.56\times10^{-39}\ \text{cm}^3. \quad (12)$$

Case 2. V_d a Square Well

The n-p interaction in odd parity states is taken to be that (scalar) square well which is appropriate to the deuteron ground state:

$$V_d(r)=\begin{cases}-V_0=-33.73\ \text{Mev} & r\leqq a=2.100\times10^{-13}\ \text{cm},\\ 0 & r>a.\end{cases} \quad (13)$$

With $\psi_0=\psi_S$, Eq. (6) becomes

$$\left\{-\frac{\hbar^2}{2\mu}\nabla^2+V_d(r)-E_0\right\}\phi_S^{(2)}=\frac{e}{2}z\psi_S. \quad (14)$$

Equation (14) can be solved by setting[6]

$$\phi_S^{(2)}=f(r)\cos\theta. \quad (15)$$

With Eq. (15), Eq. (14) yields

$$\left\{\frac{d}{dr}r^2\frac{d}{dr}-\frac{2\mu}{\hbar^2}r^2V_d(r)-\gamma^2r^2-2\right\}f(r)=-\frac{e\mu}{\hbar^2}r^3\psi_S(r). \quad (16)$$

Equation (16) can be solved for $f(r)$ by means of a one-dimensional Green's function $g(r,r')$:

$$f(r)=-\frac{e\mu}{\hbar^2}\int g(r,r')r'^3\psi_S(r')dr'. \quad (17)$$

The Green's function for Eq. (16) is[7]

$$g(r,r')=-\frac{\gamma}{1.48659}U_{\rm I}(r_<)U_{\rm II}(r_>). \quad (18)$$

$r_<$ is the smaller of r, r'; $r_>$ is the larger.

$$U_{\rm I}(r)=\begin{cases}j_1(\rho r) & r\leqq a,\\ -1.970706ij_1(i\gamma r)+0.0274676n_1(i\gamma r) & r>a,\end{cases}$$
$$U_{\rm II}(r)=\begin{cases}j_1(\rho r)-5.59266n_1(\rho r) & r\leqq a,\\ -0.765008i[j_1(i\gamma r)+in_1(i\gamma r)] & r>a.\end{cases} \quad (19)$$

j_1 and n_1 are spherical Bessel functions; $\rho^2=\gamma^2[(V_0/\epsilon)-1]$. Since V_d is not exact, it seems best to express $\phi_S^{(2)}$ in such a way that the influence of the potential is manifestly small. This can be done by solving Eq. (14) directly for $\phi_S^{(2)}$:

$$\phi_S^{(2)}=(e/2)\int G_f(\mathbf{r},\mathbf{r}')z'\psi_S(r')d\tau'-\int G_f(\mathbf{r},\mathbf{r}')V_d(r')\phi_S^{(2)}(\mathbf{r}')d\tau'. \quad (20)$$

The first term on the rhs of Eq. (20) is $\phi_S^{(1)}$, which was calculated for Case 1; in the second term, the $\phi_S^{(2)}$ to be used is given by Eqs. (15) and (17). Thus

$$\phi_S^{(2)}=\phi_S^{(1)}+\frac{e\mu}{\hbar^2}\int G_f(\mathbf{r},\mathbf{r}')V_d(r')\times\cos\theta'\left\{\int g(r',r'')r''^3\psi_S(r'')dr''\right\}d\tau'. \quad (21)$$

[6] H' connects the S state only with P states.

[7] This one-dimensional Green's function was calculated for a square well with $\rho a=1.830600$ and $\gamma a=0.4865936$. The Wronskian of the functions $U_{\rm I}$ and $U_{\rm II}$ which are given in Eq. (19), calculated for $r<a$, agrees with that calculated for $r>a$ to six figures.

Since $V_d(r')=0$ for $r'>a$, the r'' integral in Eq. (21) need only be evaluated for $r'\leqq a$. In the r'' integral, which was evaluated exactly, the term which arises from the $e^{-(\gamma+\beta)r''}$ term of ψ_S is small[8] compared to that which arises from the $e^{-\gamma r''}$ term of ψ_S for $r'\leqq a$. This small contribution was neglected in the subsequent τ' integration. For the τ' integration, the integrand was expanded in a power series, whose values differed from those of the original expression by less than 1 percent for $r'\leqq a$. With the resulting $\phi_S^{(2)}$, Eq. (7) yielded[9]

$$a_{SS}^{(2)}=a_{SS}^{(1)}+\delta a_{SS}, \quad \delta a_{SS}=0.020\times10^{-39}\ \text{cm}^3. \quad (22)$$

The author is indebted to Professor L. I. Schiff for suggesting this problem and for his guidance throughout its solution.

[8] The ratio of the term which arises from $e^{-(\gamma+\beta)r''}$ to that which arises from $e^{-\gamma r''}$ is -0.112 at $r'=0.10a$, -0.061 at $r'=0.50a$, and -0.032 at $r'=a$. The contribution of this term to δa_{SS} would be about -0.001×10^{-39} cm^3. With this estimate, Eq. (22) would read $\delta a_{SS}=0.019\times10^{-39}$ cm^3.

[9] *Note added in proof.*—J. Sawicki, Acta phys. Polon. **13**, 225 (1954), has used a different variation technique to obtain $a_{SS}\approx0.32\times10^{-39}$ cm^3. His method yields a lower limit for a_{SS}.

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Derivation of the Feynman-Dyson Rules from Time-Independent Theory

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The Feynman-Dyson rules for computing the scattering matrix are derived starting with the time-independent Schrödinger equation. Although no essentially new results are obtained, it is interesting to trace the connection between the time-dependent and time-independent methods starting from the time-independent end rather than, as is usually done, starting from the time-dependent interaction representation. In particular, a theorem due to R. J. Eden plays an important role in our discussion.

I. INTRODUCTION

THE Feynman-Dyson rules[1] for the calculation of scattering matrix elements differ from the rules of the older formulations of perturbation theory in two essential ways: (A) One can immediately write down the net contribution of all virtual processes which can be represented by the same "Feynman diagram" whereas in the older theory each virtual process was treated separately. (B) Not only is momentum conserved at each "vertex" (as in the older theory), but also energy is conserved at each "vertex."

These rules were originally derived by Dyson[1] from the time-dependent Schrödinger equation in the interaction representation, and by Feynman[1] from his Lagrangian formulation of quantum mechanics. In this note we will derive the Feynman-Dyson rules starting from the time-independent Schrödinger equation. We feel that this derivation may be of interest for two reasons: (i) It is hoped that the derivation of the Feynman-Dyson rules from the time-independent Schrödinger equation for problems in the continuum may suggest ways of further clarifying the connection between the "relativistic two-body equation"[2] and the time-independent Schrödinger equation for bound states. (ii) Our work may also be considered as a contribution to the discussion[3] of the connection between the Feynman-Dyson and the time-independent definitions of the scattering matrix. Our approach is different from that of most authors in that we start from the time-independent theory rather than from the time-dependent theory, and although no essentially new results are obtained in this way it does seem of interest to look at the connection from the "other end." In particular, we will find that a theorem due to Eden[4] will play an important role in our discussion.

In the next section we will carry through a derivation of the Feynman-Dyson rules and in the final section we will make a connection with the "adiabatic switch-on, switch-off method."[5]

II. DERIVATION OF THE FEYNMAN-DYSON RULES

The state vector for the time-independent scattering problem with interaction V satisfies the well-known equation:[6]

$$\psi=\phi-2\pi i\delta_+(E-H_0)V\psi, \quad (1)$$

where $H_0\phi=E\phi$, and where

$$\delta_+(x)=\tfrac{1}{2}\delta(x)-\text{p.v.}\frac{1}{2\pi ix}, \quad (2)$$

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