Analytic wave function for the deuteron D state*

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For calculations involving the deuteron S-state wave function it is common to use the asymptotic form for a rough approximation and the *ad hoc* Hulthén form for a better estimate. The two parameters of the Hulthén function are determined by the deuteron binding energy and the singlet effective range. In like manner we propose an *ad hoc* analytic form for the D-state wave function, which contains two parameters which are determined by the deuteron quadrupole moment and D-state percentage. The resultant function coincides very closely with the functions obtained from several widely used potential models. Since the chief value of such an analytic wave function is to calculate matrix elements quickly and easily we explicitly calculate a form of integral that allows a large class of matrix elements to be evaluated immediately.

$$\left[\text{NUCLEAR STRUCTURE } {}^2\text{H } D\text{-state wave function, calculated electromagnetic moments.}\right]$$

I. WAVE FUNCTIONS

The Hulthén wave function

$$u(r) = N(e^{-\gamma r} - e^{-\beta r}), \quad \beta \gg \gamma \tag{1.1}$$

is widely used to represent the deuteron S-state wave function. Basically the justification for this form is that the term $e^{-\beta r}$ modifies the asymptotic form $e^{-\gamma r}$ at small distances in such a way that $u(0) = 0$, and more specifically $u \sim r$, as is reasonable for S waves.[2] Moreover the parameters γ and β are not arbitrary; γ is given in terms of the deuteron binding energy ϵ and nucleon mass M as[3,4]

$$\gamma = \sqrt{M\epsilon} = 0.2316 \, \text{fm}^{-1} \tag{1.2}$$

and β may be determined from the triplet effective range parameter $r_0 = 1.75$ fm as approximately[1,5]

$$\beta = \frac{(3 - \gamma r_0) + (\gamma^2 r_0^2 - 10\gamma r_0 + 9)^{1/2}}{2r_0} = 5.98\gamma. \tag{1.3}$$

Similarly the normalization constant N may be expressed in terms of the effective range as

$$N^2 = \frac{2\gamma}{1 - \gamma r_0} = 0.783 \, . \tag{1.4}$$

For many potential models the wave functions coincide very closely with the simple Hulthén function, except of course in the region $r \lesssim 0.5$ fm where many potentials have a hard core (Fig. 1.)[6-9]

Historically the Hulthén function has been so often used in calculating deuteron matrix elements that it would be hopeless to give a list of references. However, so far as we know, no function of comparable simplicity is in common use for calculating D-state effects. We have felt the need of such a function in the past when studying the deuteron magnetic form factor,[10,11] radiative np capture,[5,12] and recently the controversial process of doubly radiative np capture $n + p \rightarrow d + 2\gamma$.[13-18]

As is well known the asymptotic form of the D-state wave function is[3,4]

$$w_A(r) = \eta N e^{-\gamma r}\left(1 + \frac{3}{\gamma r} + \frac{3}{\gamma^2 r^2}\right), \tag{1.5}$$

where η is termed the asymptotic D/S ratio, and is found to be about 0.026 in many potential mod-
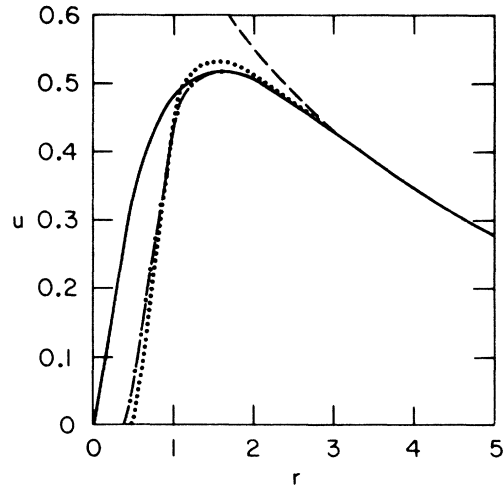

FIG. 1. S-state wave functions: Reid hard core ..., Hamada-Johnston -·-, Hulthen —, asymptotic ---.

els.[6-9] Unfortunately the tensor force has a large effective range and the wave functions obtained from potentials approach this asymptotic form very slowly, i.e., for $r \gtrsim 4$ fm (see Fig. 2). Moreover the behavior at small r is $w \sim r^{-2}$ as opposed to $w \sim r^3$ as we would expect for a D state.[2] Thus the asymptotic form is an extremely bad approximation.

To remedy this we multiply the asymptotic form by an interpolating factor which behaves like r^5 at small r and like 1 at large r. We choose explicitly

$$w(r) = \eta N(1 - e^{-\tau r})^5 e^{-\gamma r}\left(1 + \frac{3}{\gamma r} + \frac{3}{\gamma^2 r^2}\right) \qquad (1.6)$$

which clearly displays the desired limits. The parameter γ is the same as appears in (1.2), while we will treat η and τ as arbitrary parameters to be determined by experimental properties of the deuteron.

II. INTEGRALS AND PARAMETERS

The form (1.6) is surprisingly easy to handle when doing integrals, despite the occurrence of a fifth power in the interpolating factor. We will obtain the necessary integral formulas to calculate all matrix elements of the form

$$\int_0^\infty f e^{-\sigma r} r^b g\, dr\,, \qquad (2.1)$$

where f and g are either the u or w wave functions, and p is either a positive or negative integer. It is clear from the functional forms of u and w in (1.1) and (1.6) that we need to evaluate only

$$I(\lambda, \tau, n, m) = \int_0^\infty (1 - e^{-\tau r})^n \frac{e^{-\lambda r}}{r^m}\, dr \qquad (2.2)$$

for positive and negative integral values of m. Observe that we must have $n \geq m$ in order that the integrals converge. By differentiating with respect to τ we find the recursion relation

FIG. 2. D-state wave functions: Reid hard core ..., Hamada-Johnston - · -, Yale - · · -, present —, asymptotic - - -.

$$\partial I(\lambda, \tau, n, m)/\partial \tau = nI(\lambda + \tau, \tau, n - 1, m - 1). \qquad (2.3)$$

Since $I(\lambda, 0, n, m)$ is zero we may integrate to obtain

$$I(\lambda, \tau, n, m) = n \int_0^\tau I(\lambda + \tau', \tau', n - 1, m - 1)d\tau'\,. \qquad (2.4)$$

We now consider $n = m$ and obtain the following:

$$I(\lambda, \tau, 0, 0) = \frac{1}{\lambda}\,, \quad I(\lambda, \tau, 1, 1) = \ln\left(\frac{\lambda + \tau}{\lambda}\right). \qquad (2.4a)$$

It is now easy to show by induction that for $n \geq 1$

$$I(\lambda, \tau, n, n) = \frac{1}{(n - 1)!} \sum_{k=0}^n \binom{n}{k}(-1)^{n-k}(\lambda + k\tau)^{n-1}$$

$$\times \ln(\lambda + k\tau)\,. \qquad (2.5)$$

To obtain the general case of $n \geq m$ we split up the interpolating factor and expand part of it:

$$I(\lambda, \tau, n, n) = \int_0^\infty (1 - e^{-\tau r})^{n-m}(1 - e^{-\tau r})^m \frac{e^{-\lambda r}}{r^m}\, dr = \sum_{j=0}^{n-m}\binom{n - m}{j}(-1)^j \int_0^\infty (1 - e^{-\tau r})^m \frac{e^{-(\lambda + j\tau)r}}{r^m}\, dr$$

$$= \sum_{j=0}^{n-m}\binom{n - m}{j}\frac{(-1)^j}{(m - 1)!} \sum_{k=0}^m\binom{m}{k}(-1)^{n-k}(\lambda + j\tau + k\tau)^{m-1}\ln(\lambda + j\tau + k\tau). \qquad (2.6)$$

With the substitution of a new dummy index $g = j + k$ and the elementary relation

$$\sum_{j=0}^{n-m}\binom{n - m}{j}\binom{m}{q - j} = \binom{n}{q} \qquad (2.7)$$
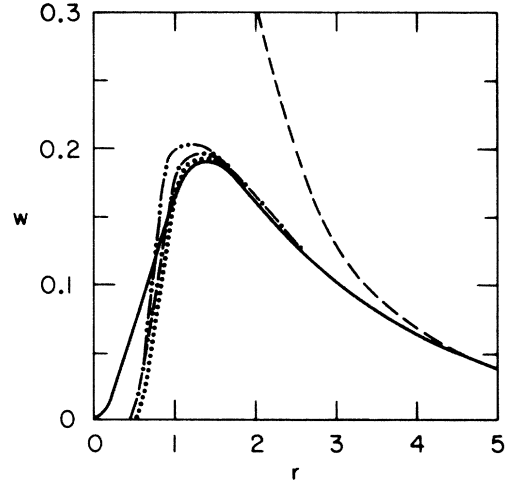
we then obtain a simple final form

$$I(\lambda, \tau, n, m) = \frac{1}{(m - 1)!} \sum_{q=0}^n \binom{n}{q}(-1)^{m-q}(\lambda + q\tau)^{m-1}$$

$$\times \ln(\lambda + q\tau), \quad n \geq m \geq 1. \qquad (2.8)$$

For m negative or zero we need only expand the

interpolating factor and use elementary integral formulas to obtain

$$I(\lambda, \tau, n, -p) = \sum_{q=0}^{n} \binom{n}{q} \frac{(-1)^q p!}{(\lambda + q\tau)^{p+1}}, \quad p \geq 0, \quad n \geq 0.$$

(2.9)

We now have evaluated the function $I(\lambda, \tau, n, m)$ for all the necessary values of n and m in (2.8) and (2.9).

Let us consider now the values of the parameters η and τ in the function w of (1.6). These may be fitted to the experimental values of the deuteron magnetic moment $\mu_D = 0.858$ and quadrupole moment $Q = 0.288$ fm^2. Since the deuteron magnetic moment may be expressed in terms of the nucleon moments $\mu_p = 2.79$, $\mu_n = -1.91$ and the D-state probability (P_D) we can equally well fit the value of P_D; explicitly the deuteron moment is given in elementary theory by[3,4]

$$\mu_D = (\mu_p + \mu_n) - \tfrac{3}{2} P_D (\mu_p + \mu_n - \tfrac{1}{2}) \tag{2.10}$$

which may be solved to give $P_D = 0.04$. There are

however additional contributions to μ_D which are not included in the above, such as meson exchange currents,[10,11,19] velocity dependent spin-orbit forces, etc.[20,21] These increase μ_D by several percent, according to estimates, and thereby increase P_D to about 0.07. This value of P_D is also in agreement with that obtained using some of the more popular potential models.[6-9] We will thus consider the two cases of $P = 0.07$ and $P = 0.04$, with the former being probably more realistic.

We now fit η and τ using the relations

$$P_D = \int_0^{\infty} w^2 dr, \quad P_D(\exp) = 0.04 \text{ or } 0.07,$$

$$Q = \frac{1}{\sqrt{50}} \int_0^{\infty} (uw - \frac{w^2}{\sqrt{8}}) r^2 dr, \quad Q(\exp) = 0.288 \text{ fm}^2.$$

(2.11)

With use of the wave functions (1.1) and (1.6) and the integral formulas (2.8) and (2.9) these reduce immediately to simple algebraic expressions.

For the D-state percentage

$$P_D = \eta^2 N^2 \sum_{n=1}^{4} \left[a_n \frac{1}{(n-1)!} \sum_{q=0}^{10} \binom{10}{q} (-1)^{n-q} (2\gamma + q\tau)^{n-1} \ln(2\gamma + q\tau) \right] + \eta^2 N^2 a_0 \sum_{q=0}^{10} \binom{10}{q} (-1)^q \frac{1}{(2\gamma + q\tau)},$$

$$a_n = \left(1, \frac{6}{\gamma}, \frac{15}{\gamma^2}, \frac{18}{\gamma^3}, \frac{9}{\gamma^4}\right) \quad (2.12)$$

and for the quadrupole moment

$$Q = \frac{\eta N^2}{\sqrt{50}} \sum_{n=0}^{2} b_n \sum_{q=0}^{5} \binom{5}{q} (-1)^q n! \left[\frac{1}{(q\gamma + 2\gamma)^{n+1}} - \frac{1}{(q\tau + \gamma + \beta)^{n+1}} \right] - \frac{\eta^2 N^2}{20} \sum_{n=0}^{2} c_n \sum_{q=0}^{10} \binom{10}{q} \frac{(-1)^q n!}{(2\gamma + q\tau)^{n+1}}$$

$$- \frac{\eta^2 N^2}{20} \sum_{n=0}^{2} d_n \sum_{q=0}^{10} \binom{10}{q} \frac{(-1)^{n-q}}{(n-1)!} (2\gamma + q\tau)^{n-1} \ln(2\gamma + q\tau),$$

$$b_n = \left(\frac{3}{\gamma^2}, \frac{3}{\gamma}, 1\right), \quad c_n = \left(\frac{15}{\gamma^2}, \frac{6}{\gamma}, 1\right), \quad d_n = \left(\frac{18}{\gamma^3}, \frac{9}{\gamma^4}\right). \quad (2.13)$$
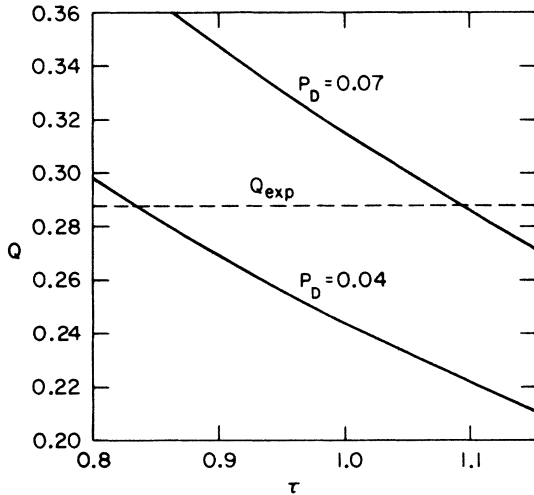
To solve these we choose a value of τ and calculate η from (2.12). These values of τ and η are then substituted into (2.13) and the resultant Q compared to the experimental value, with the final solution
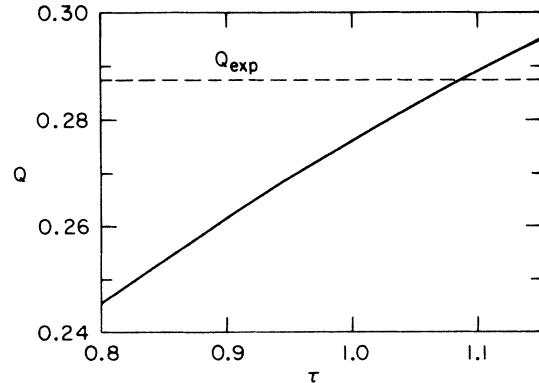

FIG. 3. Solution for the parameter τ in terms of Q exp and P_D. η is given in terms of τ from (2.12); see (2.14) and (2.15).

FIG. 4. Q as a function of τ for $\eta = 0.025$.

given by numerical interpolation.

A plot of Q versus τ is shown in Fig. 3 and we see that for $P = 0.07$

$$\tau = 1.09 \text{ fm}^{-1}, \quad \eta = 0.025 \tag{2.14}$$

and for $P = 0.04$,

$$\tau = 0.83, \quad \eta = 0.029 . \tag{2.15}$$

Not surprisingly these values of η agree quite well with that obtained with potential models, due to the fact that Q is determined largely by η and the long range behavior of the wave functions. The behavior of Q as a function of τ and η is displayed in Figs. 4 and 5.

The function w with the parameters (2.14) and (2.15) is plotted in Fig. 2 for comparison with several potential models. It is clear that for $r \gtrsim 0.5$ fm it is an excellent approximation with the $P_D = 0.07$ set of parameters.

III. SUMMARY

We have obtained a model for the deuteron D-state wave function (1.6) which is independent of dynamical considerations in the sense that no specific properties of the nuclear force are utilized. Instead the wave function is constrained to fit the percentage of D state, which is related approximately to the magnetic moment, and the deuteron
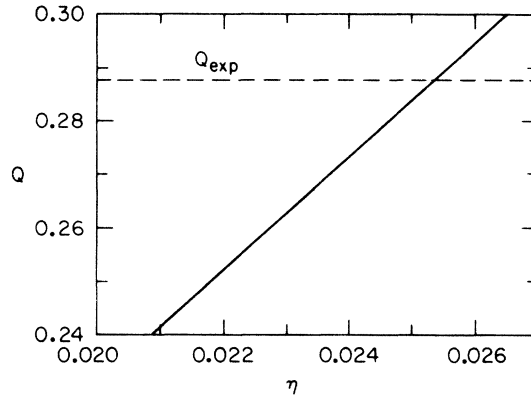

FIG. 5. Q as a function of η for $\tau = 1.09$.

quadrupole moment. A large class of integrals involving this function are readily done using the relations (2.8) and (2.9). From the graph Fig. 2 it is evident that this function is a good approximation to several widely used potential model wave functions, and because of this it is hoped that it will be a useful tool in calculating deuteron properties. In particular it should be useful in situations where a matrix element must be integrated over a parameter, e.g. second order perturbation theory for the process $n + p \to d + 2\gamma$.

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