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Measurability of the deuteron D state probability

J. L. Friar
Theoretical Division, Los Alamos Scientific Laboratory, Los Alamos, New Mexico 87545
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It is shown that several two-body unitary transformations which arise in the theory of meson-exchange currents can change the percentage D state of the deuteron, implying that this percentage is not a measurable quantity. The connection of these transformations to meson-exchange contributions to the quadrupole moment, rms radius, magnetic moment, and the asymptotic D/S ratio of the deuteron is discussed.

[NUCLEAR STRUCTURE ^{2}H; q, μ, ρ; meson-exchange currents; percent D state.]

A strict relationship between the deuteron quadrupole moment Q, the deuteron D state probability P_D, and the nucleon-nucleon tensor force has been elusive since the origins of nuclear physics, although considerable effort has been devoted to the search. A connection clearly exists, since the absence of the tensor force implies $Q = P_D = 0$; nevertheless, it has proved possible to construct diverse phenomenological potentials with widely varying values of P_D and similar values of Q. The reason for this behavior has been known qualitatively for a long time. Blatt and Weisskopf[1] argue that the quadrupole moment, given in the impulse approximation by

$$Q = \frac{1}{\sqrt{50}} \int_0^\infty r^2 Q(r)dr\,, \tag{1a}$$

$$Q(r) = u(r)w(r) - w^2(r)/\sqrt{8}\,, \tag{1b}$$

is an "outside" quantity, whose major contributions come from those values of the integrand *outside* the range of the nuclear force. This is due to the fact that the deuteron wave function $\psi_D^M(\vec{r})$, given by

$$\psi_D^M(\vec{r}) = \left[\frac{u(r)}{r} + \frac{S_{12}(\hat{r})}{\sqrt{8}}\frac{w(r)}{r}\right]\frac{\chi_M}{\sqrt{4\pi}}\,, \tag{2}$$

falls off slowly as r increases because the binding energy $\epsilon_D = 2.224\,644(46)$ MeV is very small.[2] In this equation r, u, w, S_{12}, and χ_M are the neutron-proton separation, (reduced) S- and D-state wave functions, tensor operator, and spin wave function, respectively. On the other hand, the S- and D-state probabilities P_S and P_D are defined by

$$P_S \equiv \int_0^\infty u^2(r)dr\,, \tag{3a}$$

$$P_D \equiv \int_0^\infty w^2(r)dr\,, \tag{3b}$$

where $P_S + P_D = 1$, and are "inside" quantities because they lack the extra factor of r^2 in the integrand and are sensitive to the interior region of u^2 and w^2. Presumably the deuteron mean-square radius $\langle r^2\rangle_D$ (neglecting the nucleon finite size) given in impulse approximation by

$$\langle r^2\rangle_D = \tfrac{1}{4}\int_0^\infty r^2 C(r)dr\,, \tag{4a}$$

$$C(r) = u^2(r) + w^2(r) \tag{4b}$$

is also an outside quantity. Experimentally, Q is believed to be[3] 0.2860(15) fm^2 while[4] $\langle r^2\rangle_D^{1/2} = 1.9635(45)$ fm.

Another physical quantity which is often discussed in connection with the deuteron D state is the magnetic moment μ_D, given in nuclear magnetons by

$$\mu_D = \mu_S - \tfrac{3}{2}P_D(\mu_S - \tfrac{1}{2}) + \delta_R\,, \tag{5}$$

where $\mu_S = \mu_P + \mu_N$ is the isoscalar nucleon magnetic moment, 0.8797 μ_N, and δ_R is the contribution to μ_D arising from a rich variety of relativistic and meson-exchange effects. The known value[5] of μ_D, 0.857 7406(1) μ_N, produces $P_D = 3.9\%$ if $\delta_R \equiv 0$. The recognition of the fact that exchange effects are comparable to the effect of P_D in Eq. (5) led to substantial work on the magnetic moment problem, about 25 years ago, by Breit[6] and others[7]; this work was inconclusive. Thus, folklore considers μ_D to be an inaccurate gauge of P_D.

Although relativistic and exchange corrections to μ_D have considerable antiquity, quantitative discussions of such effects in connection with the charge density, $\langle r^2\rangle_D$ and Q are more recent.[7,8] The sizes of these corrections to the impulse approximation are comparable, being a few percent. The reason is that such contributions to the charge density and to the isoscalar current density are corrections of relativistic order $(v/c)^2$. A rough estimate of all such relativistic effects is given by the relativistic correction to the nonrelativistic kinetic energy and is typically a percent to a few percent.

An additional quantity whose importance has been recognized lately[9–11] is ρ_D or η, the asymptotic D to S ratio *outside the range of the nuclear force*. This is a *true* outside quantity and is obtained by analytically continuing scattering amplitudes into the unphysical region. Its value is believed[11] to be 0.026 ± 0.002.

It is important to note that each of the quantities we have mentioned ($\epsilon_D, \langle r^2\rangle_D, Q, \mu_D, \eta$) corresponds to a well-defined specific measurement, either scattering or the interaction of the deuteron with an electromagnetic field, and these quantities necessarily include the effect of relativity and meson degrees of freedom. It has been hoped that P_D could be similarly measured by some physical process. Although values of P_D have been generated ranging from 3–9% using a wide variety of schemes, it has been felt that this disparity is the result of incompletely understood reaction mechanisms. Thus P_D remains elusive.

Bounds exist for P_D, however. Levinger[12] obtained a variational lower bound for P_D, which assumed the impulse approximation for Q. He found $P_D \geq 0.45\%$. Recently Klarsfeld[13] improved this estimate by constraining the potential to have a one-pion exchange potential (OPEP) form for $r > R$, where $R \cong 2$ fm, and found $P_D \geq 3.3\%$. This number is close to the smallest values found in some semiphenomenological potentials with OPEP tails. In spite of this apparent progress, Amado, Locher, and Simonius[9] have recently stated that P_D is not an observable of the deuteron and should be classified as a *calculated* rather than a *measured* property. Rather, they view ρ_D as a measure of the D state. A similar point of view was expressed by Amado earlier.[14] Does, then, the deuteron percentage D state have any *fundamental* meaning?

In order to answer this question we first examine a series of recent calculations of relativistic and exchange corrections to the deuteron magnetic moment[15] and charge form factor[16] carried out by the author. Within the framework of one-pion exchange *only*, a unified approach was used that allowed both pseudovector (*PV*) and pseudoscalar (*PS*) coupling of the pion to the nucleon to be treated indistinguishably. This approach has two motivations: (1) It allows the validity of the equivalence theorem (for the two couplings) to be investigated, and (2) it provides a consistency check on the method of calculation. The equivalence theorem has its origin in Dyson's[17] canonical transformation of pseudoscalar (*PS*) coupling field theory, which is transformed into pseudovector (*PV*) coupling plus additional seagull terms which violate the theorem. Suitably generalized by Drell and Henley[18] to include electromagnetism, it defines the basic vertices used in calculating exchange currents and allows motivation (1) to be realized. One actually transforms the Hamiltonian with *PS* coupling only part of the way into *PV* form using an arbitrary parameter μ ($\mu = 0$ and $\mu = 1$ correspond to *PS* and *PV*). This device allows the realization of motivation (2), since μ is an arbitrary parameter associated with the transformation. In the final results for the "dressed" nucleus with no explicit pion fields it is associated with a unitary transformation of the purely *nuclear* wave function.

We emphasize that there is *no physics* associated with this transformation and the expectation value of any operator associated with an observable (e.g., μ_D, Q) must be independent of μ. This allows a convenient check that *all* contributing processes have been calculated and calculated correctly. One of the important results of these calculations is that it is absolutely necessary to simultaneously specify every component of the matrix element of an observable: both the wave function (or equivalently the potential) and the operator. This is quite clear from the viewpoint of a unitary transformation, since both wave functions and operators are changed by such a transformation. In calculations of exchange effects of relativistic order (charge and isoscalar current operators) the unitary transformation alters the *nonstatic* parts of the one-pion-exchange potential. This fact alone casts serious doubt on all calculations of such exchange effects which use *phenomenological static* potentials. Indeed, as we shall see, it is possible in isoscalar systems to eliminate the entire exchange effect for certain observables by means of a judicious choice of μ (i.e., a choice of representation for the wave function).

As an example we present the results for the exchange corrections to charge and magnetic moment operators in an arbitrary representation. The charge form factor $F(\vec{q})$ has the basic form[19]

$$F = F_0(q) - \frac{S_{12}(\hat{q})F_2(q)}{\sqrt{8}}, \qquad (6a)$$

$$F_0{}^0 = G_E^S \int_0^\infty C(r) j_0(qr/2)\, dr, \qquad (6b)$$

$$F_2{}^0 = 2G_E^S \int_0^\infty Q(r) j_2(qr/2)\, dr, \qquad (6c)$$

$$F_0^\pi = \frac{f_0{}^2}{4Mm_\pi}\left[4G_M^S - (\mu+1)G_E^S\right] \times \int_0^\infty dr\, h_0'(r)\, q j_1(qr/2)\left[C(r) + 4\sqrt{2}\, Q(r)\right], \qquad (7a)$$

$$F_2^\pi = -\frac{f_0^2\sqrt{8}}{4Mm_\pi}\,[4G_M^S - (\mu+1)G_E^S] \times \int_0^\infty dr\, h_0'(r)[qj_1(qr/2)(C - Q/\sqrt{2}) -(27/2r)w^2 j_2(qr/2)], \tag{7b}$$

where F^0 and F^π are the conventional impulse and pion-exchange parts of F, respectively. Monopole and quadrupole parts are denoted F_0 and F_2. In addition, the wave functions (u,w) to be used in this equation are functions of μ,

$$\psi(\mu) \cong (1 - iU_E)\psi(-1)\,, \tag{8a}$$

$$U_E = -3\,\frac{f_0^2(\mu+1)}{8Mm_\pi}\,[\{\vec{\sigma}(1)\cdot\vec{p}, \vec{\sigma}(2)\cdot\vec{\nabla}h_0(r)\} + \{\vec{\sigma}(2)\cdot\vec{p}, \vec{\sigma}(1)\cdot\vec{\nabla}h_0(r)\}], \tag{8b}$$

$$u \cong u_0 + \frac{f_0^2(\mu+1)}{4Mm_\pi}\,[u_0h_0'' + 2h_0'(u_0' + \sqrt{8}w_0') + \sqrt{8}w_0(h_0'' + 3h_0'/r)] \equiv u_0 + \Delta u\,, \tag{9a}$$

$$w \cong w_0 + \frac{f_0^2(\mu+1)}{4Mm_\pi}\,[-h_0''w_0 + 2\sqrt{8}h_0'(u_0' - w_0'/\sqrt{8}) + \sqrt{8}u_0(h_0'' - 3h_0'/r)] \equiv w_0 + \Delta w\,, \tag{9b}$$

$$h_0(r) = \frac{4\pi}{m_\pi}\int \frac{d^3q}{(2\pi)^3}\,\frac{F_{\pi N}^2(q^2)e^{i\vec{q}\cdot\vec{r}}}{(q^2+m_\pi^2)} \to \frac{e^{-m_\pi r}}{m_\pi r}\,, \tag{10}$$

where the last relationship for h_0 holds if the pion-nucleon form factor $F_{\pi N}$ is identically one. We have defined $f_0^2 = f^2m_\pi^2/4\pi = 0.079$ and $f = g/2M$, while G_E^S and G_M^S are the isoscalar electric and magnetic nucleon form factors with $G_E^S(0) = 1$ and $G_M^S(0) = \mu_S$. All the form factors are functions of the momentum transfer $\vec{q}$, the j_n are ordinary spherical Bessel functions, and M and m_π are the nucleon and pion masses. We find, furthermore, that[15]

$$\delta_R = \delta_R^{\,0} + \tfrac{3}{2}\left(\mu_S - \frac{1}{2}\right)\left\{\frac{\sqrt{8}f_0^2\mu}{2Mm_\pi}\int_0^\infty [uw(h_0'' - 3h_0'/r) + 2wu'h_0']dr\right\}\,, \tag{11}$$

where $\delta_R^{\,0}$ contains additional terms, independent of μ. The pseudovector coupling results can be obtained by replacing G_M^S by G_E^S in Eq. (7); $\delta_R^{\,0}$ is also different in the two cases. We note that if one uses the usual type of Born term model to calculate exchange effects, the corresponding analysis of threshold pion photoproduction strongly favors pseudovector coupling.[20] In this case $\mu = 3$ completely eliminates one-pion-exchange parts of the isoscalar charge form factor. Most calculations use $\mu = -1$. The OPEP potential V_π is simplest for $\mu = 1$, as are the *motional*[16] relativistic corrections. For the sake of consistency, we will keep terms no higher than order f_0^2 in what follows, as we did in Eqs. (7) and (8).

Using Eq. (7) the exchange contributions to the mean-square radius and quadrupole moment can be obtained in the form

$$\langle r^2\rangle_\pi = -\frac{f_0^2}{4Mm_\pi}\,[4\mu_S - (\mu+1)]\int_0^\infty dr\, rh_0'(C + 2\sqrt{8}Q)\,, \tag{12a}$$

$$Q_\pi = -\frac{f_0^2}{2Mm_\pi}\,[4\mu_S - (\mu+1)] \times \int_0^\infty dr\, rh_0'\left(u^2 - \frac{w^2}{10} - \frac{uw}{\sqrt{2}}\right). \tag{12b}$$

It is a relatively simple matter to show that insertion of u and w from Eq. (9) into Eqs. (1) and (4) results in a set of μ-dependent terms which exactly cancels the $(\mu+1)$ term in Eq. (12), as, of course, it must. More serious, however, is Eq. (11) when inserted into Eq. (5). Unless a drastic error has been made, this equation appears to depend on μ, a completely artificial parameter. The only way out of this impasse is to assume that P_D depends on μ; calculating $\Delta P_D \cong 2\int w_0\Delta w$ produces

$$\Delta P_D = \frac{f_0^2(\mu+1)\sqrt{8}}{2Mm_\pi}\int_0^\infty dr[u_0w_0(h_0'' - 3h_0'/r) + 2h_0'w_0u_0'] \neq 0\,. \tag{13}$$

Thus we see that P_D *is not invariant under the unitary transformation* U_E. Furthermore, the μ dependence in P_D from Eq. (13) exactly cancels the μ dependence in δ_R in Eq. (11). The meson-exchange correction δ_R not only complicates the analysis of μ_D in terms of P_D, but for a subset of terms *it is indistinguishable from* P_D. Since there is no physics in a unitary transformation, we must conclude that P_D *is not a measurable quantity*, in contrast to $\langle r^2\rangle_D$, Q, μ_D, ϵ_D, and η. We have demonstrated that the first three of these quantities are μ independent and it is clear that ϵ_D must be, since to order f_0^2 the change in the Hamiltonian H produces an energy shift $\langle[U,H]\rangle \equiv 0$, independent of the form of U which we use. Furthermore, η is determined from the asymptotic region outside the range of our short-range (actually pion-range) transformation and is therefore unchanged; the same argument applies to the nucleon-nucleon phase shifts. For the same reason, $\int w^2dr$ cannot be made to vanish since w does not vanish in the asymptotic region.

This result is so clearly at variance with most of the accepted beliefs[21] that additional comment and discussion and some numerical work are warranted. Our first remark is that the conclusion above is completely consistent with the remarks in Refs. 9 and 14. In addition, since the transformation U_E changes the short-range behavior of the wave function and is of relativistic order [i.e., $(v/c)^2$], it is fair to say that P_D has both a relativistic component and is to some extent a measure of the off-shell properties of the appropriate nucleon-nucleon applitudes. This remark is bolstered if we calculate the change in Q, $\langle r^2\rangle_D^{1/2}$, and P_D produced by changing μ by 2 and choose Reid soft core (RSC) wave functions for u_0, w_0. There is no motivation for this choice other than convenience, since the RSC potential is static (local) in each partial wave. For a point π-N form factor one finds $\Delta\langle r^2\rangle_\pi^{1/2} = -0.003$ fm, $\Delta Q_\pi = -0.006$ fm^2, and $\Delta P_D = +1.7\%$; that is, since Eq. (12) gives positive results for $\mu = -1$, increasing μ decreases the resulting correction. Alternatively, if one inserts Eq. (9) into Eqs. (1) and (4) and ignores the exchange corrections, increasing μ *increases* $\langle r^2\rangle_D$, Q, and P_D, as one might expect.

The particular numbers which result are largely irrelevant to our discussion, although a 2% change in P_D is large. It is possible to lower those numbers by means of the π-nucleon form factor; in addition our arguments involve only one-pion exchange and ignore higher-order terms. Using a monopole form factor with a mass of 1 GeV produces only a slight change in $\langle r^2\rangle_\pi$ and Q_π while lowering ΔP_D to 1.3%. The reason is that the form factor affects primarily the small-r behavior. A smaller mass, such as that suggested by analysis[22,23] of the Goldberger-Treiman relation, is inexplicable from the point of view of those physical processes which might be expected[24] to generate the form factor. The integrand of ΔP_D in Eq. (13) has a maximum at about 1 fm using the form factor discussed above. This is certainly well within the range of other more complicated processes whose potentials will also possess similar unitary ambiguities; these may tend to increase or decrease ΔP_D. Our only point is that a rather small (unitary) adjustment of V (and ψ) can produce rather large fractional changes in P_D.

In order to see this, imagine that w_0 can be written as $\sqrt{P_D}v(r)$, where $\int v^2(r)dr$ is unity, and that some unitary transformation of tensor (S_{12}) character $\lambda\hat{O}$ operating on u_0 produces a change in w given by $\lambda\hat{O}u_0 = \Delta w = \lambda v(r)$. One finds immediately that $\Delta P_D \cong 2\sqrt{P_D}\lambda$. Assuming P_D ranges from 4% to 9%, one obtains $\sqrt{P_D}$ ranging from 0.2 to 0.3, and using an average value of $\frac{1}{4}$ we see that a value of 0.02 for λ produces a 1% change in P_D. From this schematic argument we see that a small transformation can produce a large fractional change in ΔP_D.

One may also ask if there are any additional unitary transformations which arise in a "natural" way similar to the way U_E arose. The answer is yes and can be found in Ref. 16. Various ways of treating retardation in meson exchanges exist and these are unitarily equivalent. One such transformation is obtained from Eq. (103a) of Ref. 16,

$$U_D = -\frac{1}{8M}\{\vec{p}; \vec{r}V_\pi\}. \tag{14}$$

It induces changes in Q and $\langle r^2\rangle_D^{1/2}$ of magnitude 0.002 fm^2 and 0.002 fm, respectively, using the previous parameters; these are similar to results found earlier. The change in P_D, however, is only 0.1%; the much smaller result can be traced to a node in Δw in the region where large contributions to ΔP_D could ordinarily be expected.

Both U_E and U_D have similar intrinsic size and both are Hermitian, even under a parity transformation, and odd under a time-reversal transformation. The latter property is important since, for any transformation, iU must be even under time reversal if the time-reversal properties of the Hamiltonian and electromagnetic current operators are to be maintained. For the two-body system in its center of mass, this means that U must be momentum dependent. Using the spins $\vec{\sigma}(1)$ and $\vec{\sigma}(2)$, and the vector $\vec{r}$ in a bilinear fashion to form a tensor operator, one cannot make an operator which is Hermitian and odd under time reversal. Using an odd number of factors of $\vec{p}$ makes this possible while maintaining parity properties.[25]

It is obvious at this point that an arbitrary unitary transformation of arbitrary strength and (finite) range can be constructed which can change P_D, since the latter quantity is not an observable (i.e., measurable). That this is not done is a result of our theoretical prejudices which *can and should be used to restrict* P_D by *fixing* the (unitary) representation. Assuming that the tail of the potential has the standard OPEP form allowed Klarsfeld to make stronger statements about P_D than Levinger could. This amounts to fixing the representation. Drastic changes in the Hamiltonian by means of a totally artificial unitary transformation would make correspondingly drastic changes in other operators, such as the magnetic moment, etc. We have attempted to introduce unitary transformations in a way which is less artificial; indeed, different methods of calculating operators of relativistic order will in general lead to different, but unitarily equivalent, results. The transformation U_E arose in just this way.

Can the representation be further restricted to eliminate the ambiguity associated with U_E? Regrettably, no representation seems uniquely best. Choosing $\mu=1$ in U_E produces the simplest potential and (motional) relativistic corrections, while the charge density is simplest for $\mu=3$. The commonly used $\mu=-1$ has no redeeming features of which we are aware. Similarly, the two representations in Ref. 16 which correspond to using or not using U_D correspond to a simpler potential and a simpler charge operator, respectively. Our own prejudice is that the potential should be simplest. Nevertheless, in view of the fact that isoscalar one-pion-exchange contributions can be eliminated from ρ by a *choice* of μ, one should be wary of statements that such contributions are needed to understand the ^{4}He and ^{3}He-^{3}H charge form factors, because structure calculation cannot reproduce certain features of these form factors. Finally we note that lower bound proofs for P_D *implicitly* assume $\mu=3$, because they *explicitly* assume impulse approximation. Thus, changing representations from $\mu=3$ to $\mu=1$ or -1 would *reduce* the minimum value of P_D, since it increases the amount of exchange contribution to Q.

We wish to emphasize that the transformation U_E arose from a field theory transformation, and a covariant treatment of the deuteron would presumably have the same problems in defining P_D as a nonrelativistic treatment has. In essence, the Dyson transformation rearranges the way pions interact with nucleons, and when the pion fields are "embedded" into the "dressed" deuteron ground state, different amounts of these fields end up in the S and D states. In this regard we note that Gross's covariant calculation of deuteron properties[26] uses a linear combination of PS and PV couplings, and finds that P_D is much more sensitive to the particular combination that is used than are Q, $\langle r^2\rangle_D$, etc. His calculation, unlike ours, does not use perturbation theory and a direct comparison is difficult. To first order in $f_0{}^2$, however, our method is equivalent to using a linear combination of PS and PV couplings specified by the parameter μ, and is thus very similar to what Gross uses.

From the point of view of relativistic corrections, the changes in Q, $\langle r^2\rangle_D$, and μ_D produced by U_E are consistent with our estimate of the size of such corrections; the effect of P_D on μ_D is also the same size. Our result that $\Delta\mu_D$ ($\equiv\delta_R$) and ΔP_D are indistinguishable for certain processes extends to heavier isoscalar systems, as well. In particular, there is a relatively small discrepancy in the isoscalar ^{3}He-^{3}H magnetic moment $\mu^{(S)}$ similar to that of the deuteron. The formula for $\mu^{(S)}$ in terms of the trinucleon D-state probability $P(D)$ is

$$\mu^{(S)}=\mu_S-2P(D)(\mu_S-\tfrac{1}{2})+\delta_R\,, \tag{15}$$

where we have lumped the S' and S-state probabilities together and used $P(S)+P(S')+P(D)=1$. The results of all the Faddeev and variational calculations that we could find for a wide variety of potentials were compiled and plotted; we found that almost all of the calculations were (approximately) consistent with

$$P(D)=\tfrac{10}{7}P_D\,. \tag{16}$$

Thus the isoscalar three-body magnetic moment problem is closely coupled to the corresponding deuteron problem and our previous remarks apply.

Finally we hypothesize that the many attempts to determine P_D experimentally have used theoretical assumptions in the analysis which have implicitly assumed a wide spectrum of reasonable representations and thus have achieved a wide variety of numbers. This may explain why P_D has remained so elusive for such a long time.

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