

Application of the constituent quark nucleon-nucleon interaction to the deuteron

S. A. Williams and F. J. Margetan

Department of Physics, Iowa State University, Ames, Iowa 50011

P. D. Morley

KMS Fusion, Inc., P.O. Box 1567, Ann Arbor, Michigan 48106

D. K. Pursey

Department of Physics, Iowa State University, Ames, Iowa 50011

(Received 18 September 1989)

The nonlocal Schrödinger equation for the two-nucleon potential derived from the interaction between constituent quarks is applied to calculating the ground state properties of the deuteron, using quark parameters consistent with single baryon data. We conclude that the two-nucleon nonlocal equation affords a very decent description of the deuteron.

I. INTRODUCTION (Ref. 1)

In the preceding paper² hereafter referred to as I, we presented our development of the nucleon-nucleon interaction derived as the residue of the color interaction between quarks. Whereas the scale of the unscreened color force seen within a hadron is m (quark mass) $\sim \Lambda_{\text{QCD}} \simeq 200$ MeV, we found that the surviving colorless interaction between two nucleons goes as overlap integrals $\times m$, which makes the scale of the order of MeV. As demonstrated in I, there is an effective exchange of quarks which occurs in the full application of the Pauli principle to the six-quark problem and only the exchange terms among the quarks contribute to the nucleon-nucleon interaction. The quark-quark potential energy used in I was the short range one-gluon exchange and the long-range linear confinement. We refer here to the derived *nucleon-nucleon potential* as U_{OGE} , with the subscripts meaning that the full one-gluon plus confinement terms were used. It is the purpose of this paper to report the application of U_{OGE} to the calculation of the energy, quadrupole moment, rms radius, and magnetic dipole moment of the deuteron.

We noted in I that to reduce the computational details we replaced the exact nucleon three-quark state function³ (which is very complicated) by a simple Gaussian approximation with spin and isospin decoupled from the orbital angular momentum. There are in U_{OGE} four parameters: α_s , the strength of the short-range gluon exchange interaction; m , the common up-quark, down-quark mass; β , the intrinsic length of the internal nucleon function; and k , the strength of the long-range linear confinement. Had we derived the nucleon-nucleon interaction using the exact internal nucleon wave function, these would all be fixed by the baryon properties as is done in the work of Kiefer.³ Since we have not used the exact internal nucleon wave function, we fit β to the size of the nucleon

consistent with the approximate starting Gaussian. Furthermore, also consistent with that function, m is fixed by the nucleon magnetic moment. We choose k to be a value consistent with the single baryon work;³ the nuclear potential and the deuteron properties are quite insensitive to k . Finally we determined α_s , from the two-nucleon data subject to its value not being vastly different from that appropriate to the exact nucleon wave function.

In Sec. II we shall discuss the diagonalization procedure necessitated by the fact that U_{OGE} is nonlocal; some details of the necessary generalized Brody-Moshinsky⁴ brackets are relegated to the Appendix. In Sec. III we shall detail the modifications necessary in the deuteron magnetic dipole and electric quadrupole operators to account for the internal structure of the nucleons. In Sec. IV we present our results.

II. DIAGONALIZATION

The general form of the nonlocal nucleon-nucleon equation is given as Eq. (1) in I. It has the form

$$\int d^3r' H(\mathbf{r}, \mathbf{r}') \psi_j(\mathbf{r}') = E_j \int d^3r' K(\mathbf{r}, \mathbf{r}') \psi_j(\mathbf{r}'), \quad (1)$$

where

$$H(\mathbf{r}, \mathbf{r}') = \frac{P^2}{M} \delta^3(\mathbf{r} - \mathbf{r}') + U(\mathbf{r}, \mathbf{r}'). \quad (2)$$

In Eq. (2) \mathbf{P} is the momentum conjugate with internucleon distance \mathbf{r} , M is the nucleon mass and $U(\mathbf{r}, \mathbf{r}')$ is the nonlocal potential which we said we will call U_{OGE} . The two-nucleon function, $\psi_j(\mathbf{r})$, appears in the 6-quark wave function² and depends on the 6-quark {total spin, total isospin} = $\{S, T\} = \{j\}$ quantum numbers. The normalization kernel, $K(\mathbf{r}, \mathbf{r}')$, is given in the Appendix and the normalization condition on $\psi(\mathbf{r})$ is

$$\int d^3r d^3r' \psi_j^*(\mathbf{r}) K(\mathbf{r}, \mathbf{r}') \psi_i(\mathbf{r}') = \delta_{ji}. \quad (3)$$

If one expands the $\psi_j(\mathbf{r})$ in terms of a complete set of functions $\{\zeta_\alpha(\mathbf{r})\}$, then

$$\psi_j(\mathbf{r}) = \sum_{\alpha} A_{\alpha j} \zeta_{\alpha}(\mathbf{r}) \quad (4)$$

and with this Eq. (1) becomes

$$\sum_{\alpha} H_{\beta\alpha} A_{\alpha j} = E_j \sum_{\alpha} K_{\beta\alpha} A_{\alpha j}, \quad (5)$$

where

$$H_{\beta\alpha} = \int d^3r d^3r' \zeta_{\beta}^*(\mathbf{r}) H(\mathbf{r}, \mathbf{r}') \zeta_{\alpha}(\mathbf{r}') \quad (6)$$

and similarly for $K_{\beta\alpha}$. The normalization condition Eq. (3) becomes

$$\sum_{\alpha\beta} A_{\alpha j} A_{\beta k}^* K_{\beta\alpha} = \delta_{jk}. \quad (7)$$

We may rewrite these equations in matrix form as

$$HA = KAE, \quad (8)$$

$$A^{\dagger}KA = 1. \quad (9)$$

Since Eq. (9) implies $KA = (A^{\dagger})^{-1}$, we may rewrite Eq. (8) as

$$A^{\dagger}HA = E, \quad (10)$$

where E is the diagonal energy matrix.

Since Eq. (9) does not give the usual normalization for the two-nucleon problem, we define

$$\begin{aligned} K^{1/2}A &= B, \\ B^{\dagger} &= A^{\dagger}K^{1/2}. \end{aligned} \quad (11)$$

Equation (11) is valid because, as we show in the Appendix, K is a positive-definite Hermitian operator. From Eq. (11)

$$B^{\dagger}B = 1 \quad (12)$$

so that Eq. (10) becomes

$$B^{\dagger}K^{-1/2}HK^{-1/2}B = E. \quad (13)$$

Since H is Hermitian, $K^{-1/2}HK^{-1/2}$ is also Hermitian. It is this matrix which we diagonalize.

We choose the eigenfunctions of the isotropic harmonic oscillator as a basis for the diagonalization. These are

$$\begin{aligned} \Phi_{NLM}(\mathbf{r}, B) &= \sqrt{2N!/B^3 \Gamma(N + L + \frac{3}{2})} \left(\frac{r}{B}\right)^L \exp\left(-\frac{r^2}{2B^2}\right) L_N^{\alpha} \left(\frac{r^2}{B^2}\right) \\ &= \phi_{NL}(r, B) Y_{LM}(\hat{r}), \quad \alpha = L + \frac{1}{2}, \end{aligned} \quad (14)$$

in which B is the oscillator length parameter and L_N^{α} is an associated Laguerre function.⁵ To these we couple the two-nucleon spin functions X_{SM_S} and append the isospin function X_{TM_T} . Thus our basis functions symbolically are

$$|NLSTJM_T M\rangle = [\Phi_{NL}(\mathbf{r}, B) X_S]_{JM} X_{TM_T}. \quad (15)$$

Our interest here is only in the positive parity states: the triplet $S = 1, T = 0, J = 1$ (hence $L = 0, 2$) and the singlet $S = 0, T = 1, J = 0$ (hence $L = 0$).

The contributions to $U(\mathbf{r}, \mathbf{r}')$ from the various V_{ij} terms of the short-range one-gluon exchange potential plus the long-range linear confinement can be reduced to five generic terms (see I). Each of these yields a term in $U(\mathbf{r}, \mathbf{r}')$ which is in general different. Also, each one does so in such a way that \mathbf{r} and \mathbf{r}' occur in $U(\mathbf{r}, \mathbf{r}')$ in different linear combinations. For example, in some of the terms they occur as $\mathbf{r} - \mathbf{r}'$ whereas for others they occur as $\mathbf{r} + \mathbf{r}'$. For yet others they occur as $3\mathbf{r} - \mathbf{r}'$. It

is therefore very convenient to change to new variables \mathbf{x} and \mathbf{y} defined by

$$\begin{aligned} \beta\mathbf{r} &= \frac{a}{a^2 + b^2} \mathbf{x} + \frac{b}{2(a^2 + b^2)} \mathbf{y}, \\ \beta\mathbf{r}' &= \frac{b}{a^2 + b^2} \mathbf{x} - \frac{a}{2(a^2 + b^2)} \mathbf{y}, \end{aligned} \quad (16)$$

where $\mathbf{x} = \beta(\mathbf{a}\mathbf{r} + \mathbf{b}\mathbf{r}')$ is the naturally occurring form. The choice of \mathbf{y} is made to ensure that $r^2 + r'^2$ has the form

$$r^2 + r'^2 = A\mathbf{x}^2 + B\mathbf{y}^2. \quad (17)$$

That is, there is no cross term $\mathbf{x} \cdot \mathbf{y}$. Finally, \mathbf{y} is scaled so that when $a = b = \frac{1}{2\beta}$, \mathbf{y} is the relative coordinate.

In computing the matrix elements of $H(\mathbf{r}, \mathbf{r}')$ or $K(\mathbf{r}, \mathbf{r}')$, one encounters forms like

$$\langle N'L'M'|H|NLM\rangle = \int d^3r d^3r' \Phi_{N'L'M'}^*(\mathbf{r}, B) H(\mathbf{r}, \mathbf{r}') \Phi_{NLM}(\mathbf{r}', B). \quad (18)$$

The $H(\mathbf{r}, \mathbf{r}')$ separates naturally into a function of \mathbf{x} and \mathbf{y} with at most one angular coupling between them. We therefore need to write the product of the two oscillator functions in terms of oscillator functions in \mathbf{x} and \mathbf{y} .

The transformation of Eq. (16) is a generalization of that which occurs in the two nucleon problem when one makes a shell model to relative coordinate transformation. The transformation coefficients are a generalization of the Brody-Moshinsky⁴ brackets and are given in the Appendix. The result is that

$$\Phi_{N'L'M'}^*(\mathbf{r}, B) \Phi_{NLM}(\mathbf{r}', B) = \sum_{N_1 L_1 M_1} \sum_{N_2 L_2 M_2} \langle N_1 L_1 M_1, N_2 L_2 M_2 | N' L' M', NLM; a, b \rangle \times (-1)^{M'} \Phi_{N_1 L_1 M_1}(\mathbf{x}, B_1) \Phi_{N_2 L_2 M_2}(\mathbf{y}, B_2), \quad (19)$$

where

$$B_1 = B\beta\sqrt{a^2 + b^2}, \quad B_2 = 2B\beta\sqrt{a^2 + b^2}. \quad (20)$$

By using Eq. (19) we may write Eq. (18) as

$$\langle N'L'M'|H|NLM\rangle = \sum_{N_1 L_1 M_1} \sum_{N_2 L_2 M_2} \langle N_1 L_1 M_1, N_2 L_2 M_2 | N' L' M', NLM; a, b \rangle \times J \int d^3x d^3y \Phi_{N_1 L_1 M_1}(\mathbf{x}, B_1) H(\mathbf{x}, \mathbf{y}) \Phi_{N_2 L_2 M_2}(\mathbf{y}, B_2) \quad (J = [2^3 \beta^6 (a^2 + b^2)^3]^{-1}), \quad (21)$$

in which the $H(\mathbf{r}, \mathbf{r}')$ has been separated into functions of \mathbf{x} and \mathbf{y} and J is the transformation Jacobian. The evaluation of the matrix elements is then straightforward. One has a similar expression for $K(\mathbf{r}, \mathbf{r}')$.

The sums in Eq. (19) and therefore Eq. (21) are finite, being restricted by energy and angular momentum conservation. Once the matrices of H and K are found, the diagonalization can proceed using standard techniques. Details of how to handle the $K^{-1/2}$ operator are given in the Appendix. We shall discuss the results of this diagonalization after we consider the electric quadrupole and magnetic dipole moments of the deuteron.

III. MOMENTS

The nucleon, and therefore deuteron, moments are expressible in terms of moments of the individual quarks which make up the nucleons. For a single nucleon then, the magnetic dipole operator is given by

$$\hat{\mu} = \mu_0 \sum_{j=1}^3 (\tau_{zj} + \frac{1}{6}) (\mathbf{l}_j + 2\mathbf{s}_j) \quad (22)$$

in which $\tau_{zj} + \frac{1}{6}$ is the charge operator for the j th quark whose angular momentum is \mathbf{l}_j and whose spin is \mathbf{s}_j . The unit of the moments is set by $\mu_0 = e\hbar/2mc$ in which m is the quark mass. (We consider only equal up and down quarks.)

With our internal nucleon wave function only the spin parts would contribute to the nucleon dipole moment. In

order to connect the quark mass with the nucleon mass, we shall proceed with a more general wave function, in which we explicitly do not use center of momentum coordinates. The form is

$$\Phi = \phi(\boldsymbol{\lambda}, \boldsymbol{\rho}, \mathbf{r}) |\sigma \sigma_z; \tau \tau_z\rangle |C\rangle,$$

where $\sigma = \tau = \frac{1}{2}$,

$$|\sigma \sigma_z; \tau \tau_z\rangle = \frac{1}{\sqrt{2}} \sum_J |(\frac{1}{2})^2 J \frac{1}{2} \sigma \sigma_z; (\frac{1}{2})^2 J \frac{1}{2} \tau \tau_z\rangle$$

is the symmetric spin-isospin function, and $|C\rangle$ is the antisymmetric color singlet. The function $\phi(\boldsymbol{\lambda}, \boldsymbol{\rho}, \mathbf{r})$ contains all the spatial and therefore orbital angular momentum information; it is symmetric. The internal Jacobi coordinates, $\boldsymbol{\rho}$, $\boldsymbol{\lambda}$ and the center-of-mass coordinate \mathbf{r} , are defined in I by

$$\begin{aligned} \boldsymbol{\rho} &= \frac{1}{\sqrt{2}} (\mathbf{r}_1 - \mathbf{r}_2), \\ \boldsymbol{\lambda} &= \frac{1}{\sqrt{6}} (\mathbf{r}_1 + \mathbf{r}_2 - 2\mathbf{r}_3), \\ \mathbf{r} &= \frac{1}{3} (\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3) \end{aligned} \quad (23)$$

in which the \mathbf{r}_j are the quark coordinates. Since the overall wave function is antisymmetric we may write μ as

$$\mu = \frac{3}{2} \mu_0 \sum_j \int d^3 \rho d^3 \lambda \phi^*(\boldsymbol{\lambda}, \boldsymbol{\rho}, \mathbf{r}) \left(\left(\frac{1}{2} \right)^2 J \frac{1}{2} \frac{1}{2} \frac{1}{2} |l_{3z} + 2s_{3z}\rangle \left(\frac{1}{2} \right)^2 J \frac{1}{2} \frac{1}{2} \frac{1}{2} \right) \\ \times \left(\left(\frac{1}{2} \right)^2 J \frac{1}{2} \frac{1}{2} \tau_z |(\tau_{3z} + \frac{1}{6})\rangle \left(\frac{1}{2} \right)^2 J \frac{1}{2} \frac{1}{2} \tau_z \right) \phi(\boldsymbol{\lambda}, \boldsymbol{\rho}, \mathbf{r}).$$

Now we may write

$$\left\langle \left(\frac{1}{2} \right)^2 J \frac{1}{2} \frac{1}{2} \tau_z |(\tau_{3z} + \frac{1}{2})\rangle \left(\frac{1}{2} \right)^2 J \frac{1}{2} \frac{1}{2} \tau_z \right\rangle \\ = 2\tau_z (-1)^J \left\{ \begin{matrix} \frac{1}{2} & \frac{1}{2} & 1 \\ \frac{1}{2} & \frac{1}{2} & J \end{matrix} \right\} + \frac{1}{6}.$$

Furthermore

$$\left\langle \left(\frac{1}{2} \right)^2 J \frac{1}{2} \frac{1}{2} \frac{1}{2} |s_{3z}\rangle \left(\frac{1}{2} \right)^2 J \frac{1}{2} \frac{1}{2} \frac{1}{2} \right\rangle \\ = 2(-1)^J \left\{ \begin{matrix} \frac{1}{2} & \frac{1}{2} & 1 \\ \frac{1}{2} & \frac{1}{2} & J \end{matrix} \right\} \left\langle \frac{1}{2} \frac{1}{2} |S_z| \frac{1}{2} \frac{1}{2} \right\rangle \quad (24)$$

in which $|\frac{1}{2} \frac{1}{2}\rangle$ is a single nucleon spin state and S_z is the z component of the single *nucleon* spin operator.

Then, with \mathbf{p}_3 the momentum conjugate to \mathbf{r}_3 ,

$$\mathbf{p}_3 = \frac{2}{\sqrt{6}} \mathbf{q} + \frac{1}{3} \mathbf{P}$$

in which \mathbf{q} is the momentum conjugate with $\boldsymbol{\lambda}$ and \mathbf{P} is conjugate with \mathbf{r} . Also

$$\mathbf{r}_3 = -\frac{\sqrt{6}}{3} \boldsymbol{\lambda} + \mathbf{r}, \\ l_3 = -\frac{2i}{3} (\boldsymbol{\lambda} \times \mathbf{q}) + i\frac{\sqrt{6}}{9} (\boldsymbol{\lambda} \times \mathbf{P}) + \frac{2i}{\sqrt{6}} (\mathbf{r} \times \mathbf{q}) + \frac{1}{3} \mathbf{L},$$

where $\mathbf{L} = -i(\mathbf{r} \times \mathbf{P})$ is the nucleon orbital angular momentum. In our basis the spin state couples to $\frac{1}{2}$, hence the internal state $\phi(\boldsymbol{\lambda}, \boldsymbol{\rho})$ must couple to 0 (1 being not allowed by parity). So long as the internal states involve only S states in $\boldsymbol{\lambda}$ and $\boldsymbol{\rho}$ the first term vanishes. The second and third vanish by symmetry, and upon forming the sum over J , the appropriate *single* nucleon operator is found by inspection of the matrix element to be

$$\hat{\mu} = \frac{\mu_0}{3} [(\tau_z + \frac{1}{2})\mathbf{L} + (10\tau_z + 1)\mathbf{S}]. \quad (25)$$

Equation (25) is the correct magnetic moment operator for a nucleon made up of three quarks. The spin part is that usually quoted in the literature.⁶

When Eq. (25) is set equal to the usual expression for the proton ($\tau_z = +\frac{1}{2}$) or neutron ($\tau_z = -\frac{1}{2}$), one obtains three relationships between the quark mass m and the nucleon mass M . From the neutron spin term $m = 0.348M$, while from the proton spin terms, $m = 0.358M$. From the orbital term for a proton, $m = 0.333M$.

Ideally, these should all be the same, but there are corrections which we have omitted. We have ignored a small mass difference between up and down quarks, which must be responsible for the difference between the quark masses derived from the neutron and proton spin terms. For the orbital term there will be a mass correction reflecting the fact that $M \neq 3m$. This requires a discussion similar to that given for the Hamiltonian in I, but a complete treatment needs a three-particle Foldy-Wouthousen transformation.⁷ We have not attempted a detailed resolution of this formidable problem. Thirdly, if the internal nucleon wave function includes other than S -quark states (see Kiefer³) then there will be an orbital correction term. For example, if $\boldsymbol{\lambda}$ and $\boldsymbol{\rho}$ involve $l = 2$ coupled to zero, there will be a correction. If one includes the state where $\boldsymbol{\rho}$ has $l = 2$, $\boldsymbol{\lambda}$ has 0 and vice versa, then $S = \frac{3}{2}$ must be coupled for overall nucleon spin $\frac{1}{2}$. This will alter the spin term as well. Here, and in the deuteron calculation, we content ourselves to using the average of these values, $m = 0.346M = 325$ MeV.

To determine a consistent expression for the *deuteron* magnetic dipole moment, we shall use the kernel normalized wave function of Eq. (4). The magnetic dipole moment is

$$\mu = \left\langle \mu_0 \sum_{j=1}^6 (\tau_{zj} + \frac{1}{6})(l_{zj} + 2s_{zj}) \right\rangle_{J=M=1}.$$

Since the deuteron ground state has $T = 0$, the τ_{zj} term will not contribute. Hence in vector form we have

$$\boldsymbol{\mu} = \frac{\mu_0}{6} \int d^3 \rho_A d^3 \rho_B d^3 \lambda_A d^3 \lambda_B d^3 r \psi^*(\mathbf{r}) f^* \left\langle STC \left| \sum_{j=1}^6 (\mathbf{l}_j + 2\mathbf{s}_j) [1 - 9(36)] \psi(\mathbf{r}) f |STC \right. \right\rangle \quad (26)$$

in which $\psi(\mathbf{r})$ is the *spatial* deuteron ground state wave function, \mathbf{r} is the inter-nucleon separation vector, and ρ_A, ρ_B , etc. are the Jacobi coordinates for nucleons A and B . The function f is given by the product of two harmonic oscillator functions

$$f = \phi(\boldsymbol{\lambda}_A, \boldsymbol{\rho}_A) \phi(\boldsymbol{\lambda}_B, \boldsymbol{\rho}_B),$$

where

$$\phi(\mathbf{x}, \mathbf{y}) = \frac{\beta^3}{\pi^{3/2}} \exp\left(-\frac{1}{2\beta^2}(x^2 + y^2)\right).$$

Since the wave functions have been constructed to be antisymmetric under any pair of quark exchanges we may replace Eq. (26) by

$$\mu = \mu_0 \int d^3\rho_A d^3\rho_B d^3\lambda_A d^3\lambda_B d^3r \psi^*(\mathbf{r}) f^* \langle STC | [(1_1 + 2s_1) - 3(2l_1 + l_3 + 4s_1 + 2s_3)(36)] \psi(\mathbf{r}) f | STC \rangle. \quad (27)$$

To process this equation, we express each of these operators in terms of Jacobi coordinates for nucleons A and B , their conjugate momenta, and $\mathbf{L} = \mathbf{r} \times \mathbf{P}$ in which \mathbf{P} is the momentum conjugate to \mathbf{r} . We also use Eq. (24) as well as the fact that the deuteron ground state has $S = 1$ and $T = 0$. Finally, one must use the result derivable from I that

$$f^* \langle STC | (36) | STC \rangle f = \frac{2^6 \pi^{3/2}}{3^6 \beta^3 \sqrt{3}} [\delta^3(\mathbf{r} - \mathbf{r}') - K(\mathbf{r}, \mathbf{r}')]$$

in which $\mathbf{r}' = (36)\mathbf{r}$. It is then not difficult to show that

$$\mu = \mu_N \frac{M}{6m} \int d^3r d^3r' \psi_{M_J=J=1}^{S=1, T=0*}(\mathbf{r}) K(\mathbf{r}, \mathbf{r}') \times (L'_z + 2S_z) \psi_{M_J=J=1}^{S=1, T=0}(\mathbf{r}') \quad (28)$$

in which μ_N is the nuclear magneton, M is the nucleon mass and m is the quark mass with $\mathbf{L}' = (36)\mathbf{L} = \mathbf{r}' \times \mathbf{P}'$. Here $\psi_{M_J}^{S,T}$ is the deuteron wave function including spin and isotopic spin, $\psi_{M_J}^{S,T} = \psi(\mathbf{r}) | SLJM \rangle | T_A T_B T \rangle$.

For an individual quark, the quadrupole operator is

$$\hat{q}_j = (\tau_{jz} + \frac{1}{6}) T(\mathbf{r}_j); \quad T(\mathbf{r}_j) = 3z_j^2 - r_j^2 \quad (29)$$

and the deuteron quadrupole moment operator is then

$$\hat{Q} = \sum_{j=1}^6 \hat{q}_j. \quad (30)$$

The tensorial character of the τ_{zj} terms will lead to a Clebsch-Gordan $C(T_1 T; T_0 T)$ in the expectation value of this operator and since $T = 0$ for the deuteron ground state, these terms vanish. Thus the effective operator is just

$$\hat{Q}_{\text{eff}} = \frac{1}{6} \sum_{j=1}^6 T(\mathbf{r}_j). \quad (31)$$

In computing the expectation value of this operator, we shall again use the K -normalized wave function. The antisymmetrization is as usual affected by \mathcal{P} , the projection operator which is defined in I. Because of the idempotent property of \mathcal{P} together with the $(S_3 \times S_3) \times S_2$ antisymmetry of the function upon which it acts, we may write the expectation value of Q_{eff} as

$$\begin{aligned} Q &= \frac{1}{3} \int d^3\rho_A d^3\rho_B d^3\lambda_A d^3\lambda_B d^3r \psi^*(\mathbf{r}) f^* \langle STC | [2T(\mathbf{r}_1) + T(\mathbf{r}_3)] [1 - 9(36)] \psi(\mathbf{r}) f | STC \rangle \\ &= \int d^3\rho_A d^3\rho_B d^3\lambda_A d^3\lambda_B d^3r \psi^*(\mathbf{r}) f^* T(\mathbf{r}_1) \psi(\mathbf{r}) f \\ &\quad - 3 \int d^3\rho_A d^3\rho_B d^3\lambda_A d^3\lambda_B d^3r \psi^*(\mathbf{r}) f^* \langle STC | [2T(\mathbf{r}_1) + T(\mathbf{r}_3)] (36) | STC \rangle \psi(\mathbf{r}) f. \end{aligned} \quad (32)$$

We process Eq. (32) in the manner similar with that discussed for the magnetic dipole moment and find

$$Q = \frac{3}{32} \int d^3r d^3r' \psi_{M_J=J=1}^{S=1, T=0*}(\mathbf{r}) [2T(\mathbf{r} - \mathbf{r}') + T(\mathbf{r} + \mathbf{r}')] K(\mathbf{r}, \mathbf{r}') \psi_{M_J=J=1}^{S=1, T=0}(\mathbf{r}') - \frac{1}{8} \int d^3r \psi_{M_J=J=1}^{S=1, T=0*}(\mathbf{r}) T(\mathbf{r}) \psi_{M_J=J=1}^{S=1, T=0}(\mathbf{r}), \quad (33)$$

where we have used the fact that these operators are spin-isospin independent to include the full deuteron wave function $\psi_{M_J}^{S,T}$. Once the deuteron wave function (K normalized) is determined, Eqs. (28) and (33) give the magnetic dipole and electric quadrupole moments, respectively.

IV. RESULTS

There are four parameters in the calculation: α_s , the strength of the short-range potential; k , the strength of the long-range potential; m , the common up-down quark mass; and β , where $\frac{1}{\beta}$ is the intrinsic length of the inter-

nal quark wave functions describing the nucleons. The parameters β and m are fixed: β at 243 MeV from the proton radius and m at 325 MeV from the nucleon magnetic moments. The two remaining parameters could in principle be varied freely to find the best fit to four pieces of experimental deuteron data: $E_b = 2.2$ MeV, the binding energy of the $J = 1$ ground state; $Q = 0.282e^2\text{fm}^2$, the deuteron quadrupole moment; $\mu = 0.857\mu_N$, the deuteron magnetic dipole moment; and $r_{\text{rms}} = 2.1$ fm, the deuteron root-mean-square charge radius. In practice, we found the results are insensitive to changes in k so we fixed k at 4×10^4 MeV². This value is consistent with the small basis study of the N and Δ baryon spectra by Kiefer.³ Therefore, 3 out of the 4 parameters are fixed by single baryon data [or putting it another way, by the $H(3)$ Hamiltonian]. In principle, α_s should also be determined. However, for semirelativistic quarks, α_s varies considerably with momentum transfer and its value appropriate for $H(3)$ will be different than that for $H(6)$, simply due to the difference of momenta associated with the two Hamiltonians. We compensate by permitting α_s to vary somewhat, subject to its being not grossly different from the value $\alpha_s/\pi = 0.64$ suggested by the baryon work.³

One final variable enters the calculation, but it is not a parameter. This is $p = \beta b$ where b is the intrinsic length of the harmonic oscillator basis used for diagonalization. Of course, in an infinite basis, results would be independent of the choice of p . In any finite basis there will remain some vestige of p dependence. One attempts to minimize this nonphysical dependence by choosing p in a range over which results are essentially p independent.

Our $S = 1$, $T = 0$, $J = 1$ basis states are ordered according to increasing energy and for degenerate energy, in decreasing orbital angular momentum. Table I shows the basis, up to reduced energy $20\hbar\omega$.

The search for the proper range of p is complicated by the variability of α_s . To speed up the search procedure, we first studied the energy of the ground state in a 15 dimensional basis. In Fig. 1 we show this energy as a function of p for various α_s . There are two criteria here: The calculated energy should be negative (indicating binding) and above the target energy of -2.2 MeV. Increasing basis size is guaranteed to lower the energy since diagonalization gives an upper bound. Secondly, there should be a region of p for which the calculated energy is essentially p independent. From Fig. 1 we concluded that for the one-gluon-exchange short-range plus long-range confinement (OGE), a value of α_s , between 1.7 and 1.8 (α_s/π between 0.54 and 0.57) is appropriate and p should lie between 1.5 and 2. More detailed studies in

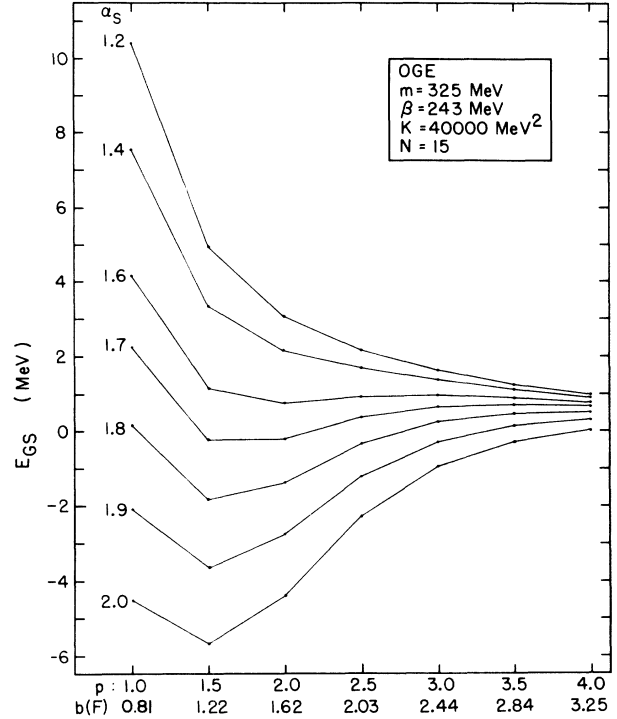


FIG. 1. Calculated ground state energies of the deuteron in an $N = 15$ basis as a function of the basis parameter $p = \beta b$, for various values of α_s . The other parameters are fixed as indicated in text.

the vicinity of the flat (p independent) minima yielded the final result $\alpha_s = 1.785$.

Our next task was to find a sufficiently large basis such that the calculated energy will have converged close to the infinite basis value. In Fig. 2 we show the calculated energy as a function of basis size for $p = 1.5$ and $p = 2$. We also show the points for $p = 1.0$ and $p = 2.5$ for up to a 15 dimensional basis. We also note that by the time $N = 21$, both the $p = 2.0$ and $p = 1.5$ curves have begun to flatten out indicating convergence to a value near to -2 MeV. We had hoped to continue the graph fully to convergence, but estimates of computer time and costs indicated that would not be cost effective; to proceed even to a 27 dimensional basis would approximately double the cost. Hence, we have used a difference procedure to estimate the converged values.

Detailed examination of the numerical values indicated that $E(J = 1)$ changes more smoothly when N is increased by 4 rather than by 2. In Fig. 3 we graph the difference $E(J = 1)_N - E(J = 1)_{N+4}$ versus N . For

TABLE I. Index assignment for the oscillator basis states $|n, L\rangle$; $(E - 3/2\hbar\omega)$ is in units of $\hbar\omega$.

| $ nL\rangle$ | $ 0, 0\rangle$ | $ 0, 2\rangle$ | $ 1, 0\rangle$ | $ 1, 2\rangle$ | $ 2, 0\rangle$ | ... | $ 9, 2\rangle$ | $ 10, 0\rangle$ |
|------------------------|----------------|----------------|----------------|----------------|----------------|-----|----------------|-----------------|
| $(E - 3/2\hbar\omega)$ | 0 | 2 | 2 | 4 | 4 | ... | 20 | 20 |
| Index N | 1 | 2 | 3 | 4 | 5 | ... | 20 | 21 |

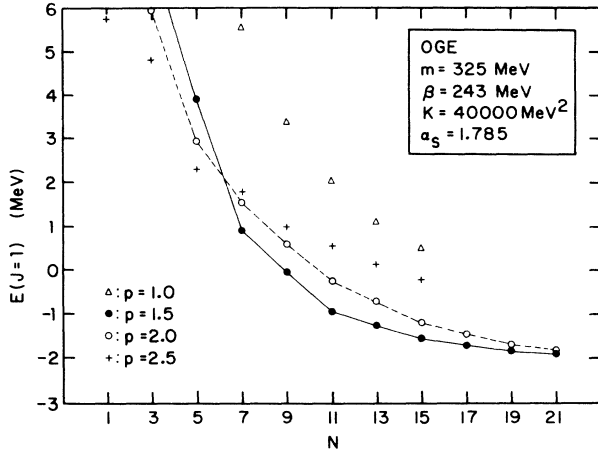


FIG. 2. Calculated ground state energy of the deuteron as a function of basis size, N , for different values of the basis parameter p . The parameters are indicated for the OGE potential.

$p = 2.0$ a rather good straight line can be drawn through the points $N = 5$ onward, while for $p = 1.5$ only the points from $N = 11$ onward fit well on a straight line. From this one can extrapolate to a converged value. If Δ_{21} is the difference between the last point and the first extrapolated point on the line, and if f is the rate of fall,

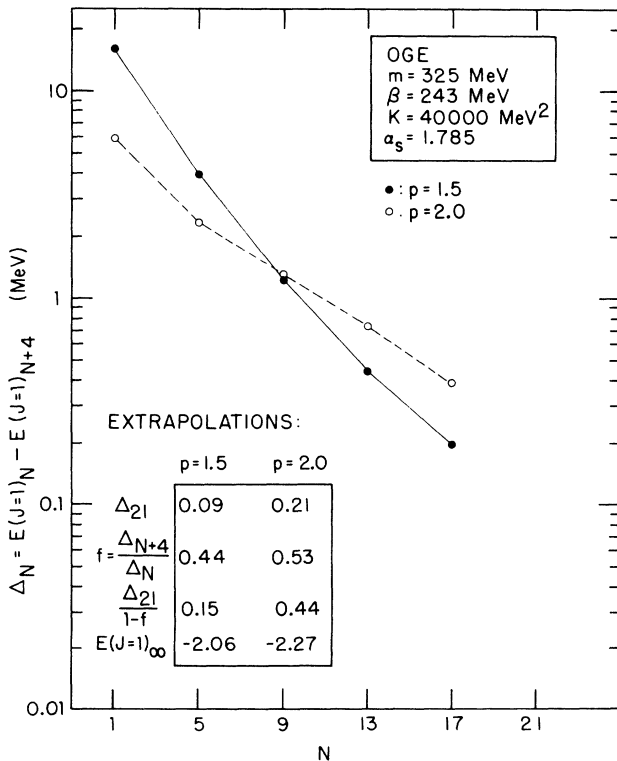


FIG. 3. Extrapolation of energy differences versus basis size. This graph is used to estimate the ground state energy in a fully converged calculation (infinite basis).

then the remaining drop is $\Delta_{21}/(1-f)$. We use this technique to estimate $E(J=1) = -2.28$ MeV for $p = 2.0$ while for $p = 1.5$ the estimated converged value is -2.10 MeV. Close analysis of the numerics indicates a slight downward curvature for the $p = 2.0$ results while for $p = 1.5$ results have a slight upward curvature. Therefore we conclude that the converged binding energy is bracketed by $2.10 \text{ MeV} < BE < 2.28 \text{ MeV}$ for the OGE potential. We remind the reader again that OGE includes the complete one-gluon exchange and linear confinement.

Just as the energy is not fully converged yet by $N = 21$, neither are the other physical quantities of interest: μ , Q , and r_{rms} . Furthermore, each of these is more sensitive to changes in basis than is the energy. Figure 4 displays the magnetic dipole moment μ as a function of N . Notice that changing the basis by 4 rather than 2 makes a smoother variation. This is undoubtedly connected with the fact that the $|2,0\rangle$ oscillator wave function is more like the $|0,0\rangle$ than is the $|1,0\rangle$. Alternative points for either $p = 2.0$ or $p = 1.5$ display very closely either rising or falling exponential behavior. From these we estimate convergence at $\mu = 0.90 \pm 0.01$. The quadrupole moment calculation displayed in Fig. 5 shows even more sensitivity to adding only 2 states to the basis. Furthermore, the quadrupole moment, being very sensitive to small contributions from higher states, is less well converged. We see, however, that for both values of p the $\Delta N = 2$ excursions are becoming less and less near $N = 21$. Here alternate points fit rather closely on curves of the form $Q_0[1 - \exp(-\xi N)]$. Using this, we estimate a converged value of $Q = 0.13 \pm 0.005$.

Of all physical quantities, r_{rms} , the root-mean-square charge radius is least well converged. The extrapolation to convergence is made from Fig. 6 data and has the largest uncertainty. We estimate a converged value of $r_{\text{rms}} = 1.8 \pm 0.2$.

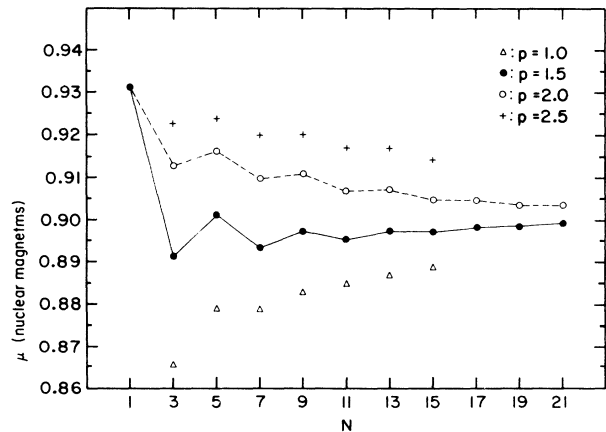


FIG. 4. Calculated ground state magnetic dipole moment values of the deuteron as a function of basis size for various values of the basis parameter p . These curves are used to estimate the magnetic dipole moment in a fully converged calculation (infinite basis).

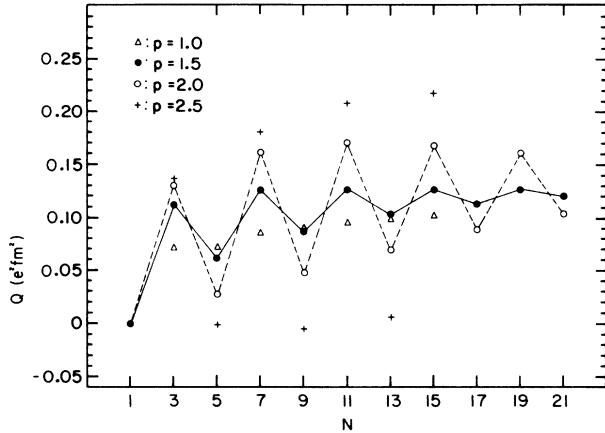


FIG. 5. Calculated ground state quadrupole moment values of the deuteron as a function of basis size for various values of the basis parameter p . These curves are used to estimate the quadrupole moment in a fully converged calculation (infinite basis).

To assess the stability of the calculation to the values of the parameters found, we repeated the $N = 21$ calculation with each parameter in turn increased and decreased by five percent, except for k for which we made ten percent changes. The results are shown in Table III. It is not surprising that the binding energy is sensitive to small changes in the parameters, since the binding energy arises as a result of cancellations between large quantities. What is surprising is that the quadrupole and dipole moments and the charge radius are astonishingly stable, as Table III shows. It is notorious that variational calculations frequently give good energies but poor wave functions. The present calculation appears to reverse this conventional wisdom since the quantities dependent on the wave function are well determined. Finally, we note

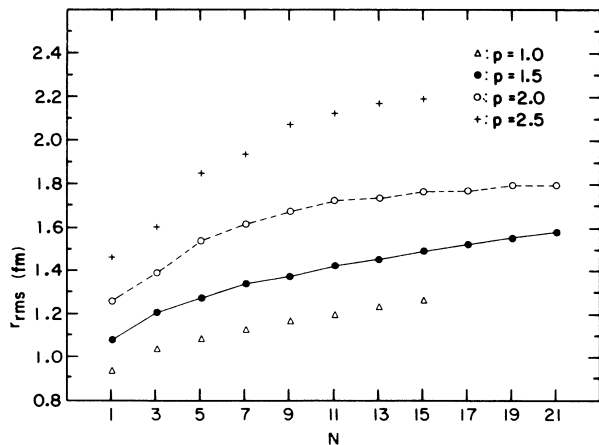


FIG. 6. Calculated ground state mean-square charge radius of the deuteron as a function of basis size for various values of the basis parameter p . These curves are used to estimate the mean-square charge radius in a fully converged calculation (infinite basis).

that for the final determination of the parameters the $E(J = 0)$ state is computed to be unbound (diagonalization of the Hamiltonian in a finite basis can establish that a state has positive energy and is therefore unbound, but the energy so found cannot be given a meaningful physical interpretation).

Of particular interest is the relative contributions of the various pieces of H to the deuteron binding energy. To find out, we have computed the $N = 21$ basis vector expectation value for each of the terms in the Hamiltonian. We shall use the term kinetic energy to refer to P^2/M ; the kinetic energy correction refers to U_0 of I. The remaining terms are detailed in I. Table IV gives the breakdown.

As expected, the central, tensor, and spin-orbit pieces provide the binding, while the other terms are antibinding. We note also the nearly negligible contribution from the quark confinement potential.

Based upon the results of Tables II, III, and IV, we conclude that the nonlocal nucleon-nucleon Schrödinger equation derived from the 6-quark Hamiltonian affords a very decent description of the two-nucleon data. To achieve this, it is necessary to (i) use the entire one-gluon-exchange potential to order v^2/c^2 , (ii) carry the kinetic energy expansion similarly to order v^2/c^2 , (iii) fully account for the Pauli principle, and (iv) use the correct treatment for the center of mass motion of the nucleon. Of the predicted deuteron quantities, only the quadrupole moment needs improvement. This comes about by noting that the contributions to the OGE tensor part of the interaction are very sensitive to higher quark orbital angular momentum components in the internal nucleon wave function, and we have ignored these.

Direct comparison between our potential (as derived in I and used here) and that of others who have considered the two nucleon problem in a similar manner is not possible because ours is a nonlocal potential in contrast to that of Harvey,⁸ and that of Maltman and Isgur.⁹ Some comparison is possible in terms of results. As indicated in I, the basic 6-quark function has an equal mixture of all three-three quark color channels, which were called hidden by Harvey and which he found necessary. In that respect our results are not different from his. Reed-Margetan¹⁰ has made a local approximation to the nonlocal potential and finds that the resultant of a series of very complicated terms leads to rather amazingly

TABLE II. Estimated converged ($N = \infty$) results. $\alpha_s = 1.785$, $m = 325$ MeV, $\beta = 243$ MeV, and $k = 4 \times 10^4$ MeV².

| Quantity | OGE | Experimental value |
|---------------------------|--------------------|--------------------|
| $BE(J = 1)$ (MeV) | $2.10 < BE < 2.28$ | 2.2 |
| Q ($e^2 \text{fm}^2$) | 0.13 ± 0.005 | 0.282 |
| μ (μ_N) | 0.90 ± 0.01 | 0.857 |
| r_{rms} (fm) | 1.8 ± 0.2 | 2.1 |
| $BE(J = 0)$ | not bound | not bound |

TABLE III. Effect of changing the parameters by $\pm 5\%$, except for k , which was changed by $\pm 10\%$. The results are for an $N = 21$ basis size. The first line is the final parameter calculation for the $N = 21$ basis. The difference between this first line and Table II is the difference in number of basis: $N = \infty$ vs $N = 21$.

| m | β | α_s | k | $E (J = 1)$ | Q | μ | r_{rms} |
|-----|---------|------------|--------|-------------|------|-------|------------------|
| 325 | 243 | 1.785 | 40 000 | -1.91 | 0.12 | 0.90 | 1.59 |
| | | 1.874 | | -3.43 | 0.12 | 0.89 | 1.51 |
| | | 1.700 | | -0.59 | 0.12 | 0.91 | 1.67 |
| | 255 | | | +0.89 | 0.12 | 0.90 | 1.69 |
| | 231 | | | -5.14 | 0.11 | 0.90 | 1.50 |
| 341 | | | | -4.02 | 0.10 | 0.90 | 1.49 |
| 309 | | | | -0.02 | 0.14 | 0.90 | 1.70 |
| | | | 44 000 | -1.88 | 0.12 | 0.90 | 1.59 |
| | | | 36 000 | -1.93 | 0.12 | 0.90 | 1.59 |

smooth potential forms. In particular, she found a momentum dependent soft repulsive core in the deuteron channel, and that is in contrast to Harvey's reported work.

Maltman and Isgur neglected the momentum and spin-orbit terms of the one-gluon-exchange potential in their work. Also, they used a quite different confinement potential. Finally, they added a phenomenological one pion exchange tail which would give their potential a much longer range than the local approximation to ours. The greatest difference between their predications for the deuteron and ours is that they predict weak binding for the singlet S state, whereas our calculation predicts that state as strictly unbound.

The reader should keep in mind the approximations we have made in this solution to the 6-quark problem. We have attempted to keep our approximations consistent by using the first order relativistic terms for both the kinetic energy and in the one-gluon-exchange potential; we have retained only the lowest internal state of the nucleon, although we corrected the two nucleon kinetic energy expression for this; and finally, as with all other authors, we have ignored the contribution of the 3-quark potential to the two-nucleon interaction. The form of the

latter suggests that its inclusion would increase the two-nucleon tensor term and the inclusion of higher orbital angular momentum states in the internal nucleon function (such as found by Keifer³) would certainly increase the tensor term as well as effectively lengthening the tail of the two nucleon potential. Both of these might be expected to improve our predicted quadrupole moment.

From the close agreement with the deuteron data, one expects the nonlocal equation to properly predict the low energy two-nucleon phase shifts (up to the pion threshold). Espinosa and Schmidt¹¹ have used the numerical deuteron wave function without any adjustment of our parameters to compute the deuteron electromagnetic form factors. Their predictions are in very good agreement with experiment. The interested reader may also obtain the $N = 21$ vector basis wave function from the authors.

This work was supported in earlier stages by U.S. DOE Contract W-7405-eng-82. We wish to express our thanks to Dr. R. S. Hansen, former Director of the Ames Laboratory, for a Directors Development Grant in latter stages which enabled us to complete this work.

TABLE IV. Expectation values in MeV of the various parts of the Hamiltonian. The ground state of the deuteron is approximated by the $N = 21$ basis vector. The two different values of p refer to the oscillator length parameter as defined in the text. The energy in Table II is the estimated $N = \infty$ converged value.

| Hamiltonian term | $p = 1.5$ | $p = 2.0$ |
|--------------------------------------|-----------|-----------|
| Kinetic energy (E_K) | 22.64 | 19.1 |
| E_K Correction | 3.59 | 3.20 |
| Momentum | 8.21 | 7.28 |
| Tensor | -12.31 | -10.21 |
| Spin orbit | -3.06 | -2.41 |
| Central | -36.40 | -32.17 |
| Spin spin | 15.16 | 13.14 |
| Confinement | 0.26 | 0.23 |
| Total $N = 21$ computed basis energy | -1.91 | -1.84 |

**APPENDIX A:
GENERAL TRANSFORMATION BRACKETS**

We want to expand the product eigenfunctions $\Phi_{NLM}(\mathbf{r}, B)\Phi_{N'L'M'}(\mathbf{r}', B)$ of

$$H = \frac{1}{2} \left(p^2 + \frac{r^2}{B^4} \right) + \frac{1}{2} \left(p'^2 + \frac{r'^2}{B^4} \right) \quad (\text{A1})$$

in terms of the product eigenfunctions of H written in new variables \mathbf{x} and \mathbf{y} . The variable \mathbf{x} has the form

$$\mathbf{x} = \beta(\mathbf{ar} + \mathbf{br}'),$$

where a and b are fixed by the naturally occurring forms in the various generic terms, V_{ij} ; (36). The second variable $\mathbf{y}(\mathbf{r}, \mathbf{r}')$ may be chosen freely. We choose

$$\mathbf{y} = 2\beta(\mathbf{br} - \mathbf{ar}')$$

so that

$$H = \frac{1}{2\beta^2(a^2 + b^2)} \left(p_x^2 + \frac{x^2}{B^4} \right) + \frac{1}{8\beta^2(a^2 + b^2)} \left(p_y^2 + \frac{y^2}{B^4} \right). \quad (\text{A2})$$

Thus $\Phi_{N_1L_1M_1}(\mathbf{x}, B_1)\Phi_{N_2L_2M_2}(\mathbf{y}, B_2)$ are also product eigenfunctions of H where

$$B_1 = \beta B \sqrt{a^2 + b^2}, \quad B_2 = 2\beta B \sqrt{a^2 + b^2}.$$

Hence we may expand

$$\begin{aligned} \Phi_{NLM}(\mathbf{r}, B)\Phi_{N'L'M'}(\mathbf{r}', B) &= \sum_{N_1L_1M_1} \sum_{N_2L_2M_2} \langle N_1L_1M_1, N_2L_2M_2 | NLM, N'L'M'; a, b \rangle \\ &\quad \times \Phi_{N_1L_1M_1}(\mathbf{x}, B_1)\Phi_{N_2L_2M_2}(\mathbf{y}, B_2). \end{aligned} \quad (\text{A3})$$

The transformation brackets in Eq. (A3) are a generalization of Brody-Moshinsky⁴ brackets. A closed form expression for these may be derived in the same manner used by Barker and Cooper¹² for the usual brackets. In fact, when $a = b = \frac{1}{2\beta}$ these reduce to the usual brackets which serves as a useful check.

Since the Φ are normalized isotropic harmonic oscillator functions given by Eq. (14), Eq. (A3) implies

$$\begin{aligned} &\langle N_1L_1M_1, N_2L_2M_2 | NLM, N'L'M'; a, b \rangle \\ &= \int d^3x d^3y \Phi_{N_1L_1M_1}^*(\mathbf{x}, B_1)\Phi_{N_2L_2M_2}(\mathbf{y}, B_2)\Phi_{NLM}(\mathbf{r}, B)\Phi_{N'L'M'}(\mathbf{r}') \\ &= \left(\frac{2^4 N_1! N_2! N! N'}{B_1^3 B_2^3 B^6 \Gamma(N_1 + L_1 + \frac{3}{2}) \Gamma(N_2 + L_2 + \frac{3}{2}) \Gamma(N + L + \frac{3}{2}) \Gamma(N' + L' + \frac{3}{2})} \right)^{1/2} \\ &\quad \times \int x^2 dx y^2 dy d\Omega_x d\Omega_y \left(\frac{x}{B_1} \right)^{L_1} \left(\frac{y}{B_2} \right)^{L_2} \left(\frac{r}{B} \right)^L \left(\frac{r'}{B} \right)^{L'} L_{N_1}^{\alpha_1} \left(\frac{x^2}{B_1^2} \right) \\ &\quad \times L_{N_2}^{\alpha_2} \left(\frac{y^2}{B_2^2} \right) L_N^{\alpha} \left(\frac{r^2}{B^2} \right) L_{N'}^{\alpha'} \left(\frac{r'^2}{B^2} \right) \exp \left(-\frac{x^2}{B_1^2} - \frac{y^2}{B_2^2} \right) Y_{L_1M_1}^*(\hat{x}) Y_{L_2M_2}(\hat{y}) Y_{LM}(\hat{r}) Y_{L'M'}(\hat{r}') \end{aligned} \quad (\text{A4})$$

with

$$\alpha = L + \frac{1}{2}, \quad \alpha' = L' + \frac{1}{2}, \quad \alpha_1 = L_1 + \frac{1}{2}, \quad \alpha_2 = L_2 + \frac{1}{2},$$

and where we have used $(r^2 + r'^2)/2B^2 = x^2/2B_1^2 + y^2/2B_2^2$ in the exponent.

A generalization of the Moshinsky addition theorem⁴ yields

$$\begin{aligned} r^{L+2K} Y_{LM}(\hat{r}) &= \pi K! \Gamma(L + K + \frac{3}{2}) \sum_{L'_1 M'_1} \sum_{L'_2 M'_2} [(2L + 1)(2L' + 1)(2L'_2 + 1)]^{1/2} \begin{pmatrix} L'_1 & L'_2 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L'_1 & L'_2 & L \\ -M'_1 & -M'_2 & M \end{pmatrix} \\ &\quad \times \sum_{\nu_1 \nu_2} \delta_{\nu_1 + \nu_2 + P, K} Y_{L'_1 M'_1}(\hat{x}) Y_{L'_2 M'_2}(\hat{y}) (-1)^M \\ &\quad \times \frac{(\alpha x)^{L_1 + 2\nu_1} (\gamma y)^{L_2 + 2\nu_2}}{\nu_1! \nu_2! \Gamma(L'_1 + \nu_1 + \frac{3}{2}) \Gamma(L'_2 + \nu_2 + \frac{3}{2})} \end{aligned} \quad (\text{A5})$$

in which

$$P = \frac{L'_1 + L'_2 - L}{2}, \quad \alpha = \frac{a}{\beta(a^2 + b^2)}, \quad \gamma = \frac{b}{2\beta(a^2 + b^2)}.$$

We expand the Laguerre functions $L_N^{L+1/2}(r^2/B^2)$ and $L_{N'}^{L'+1/2}(r'^2/B^2)$ by using

$$L_N^\sigma(t) = \sum_k \frac{\Gamma(N + \sigma + 1)(-1)^k t^k}{\Gamma(k + \sigma + 1)(N - k)! k!}.$$

We now use Eq. (A5) and perform the necessary integrations. After some algebra the desired result is found

$$\begin{aligned} & \langle N_1 L_1 M_1, N_2 L_2 M_2 | N L M, N' L' M'; a, b \rangle \\ &= \beta^3 \frac{\pi}{4} (-1)^{N_1 + N_2 + N + N'} [2^3 (a^2 + b^2)^{2N + L + 2N' + L' + 3} N_1! N_2! N! N'! \Gamma(N_1 + L_1 + \frac{3}{2}) \Gamma(N_2 + L_2 + \frac{3}{2}) \Gamma(N + L + \frac{3}{2}) \\ & \quad \times \Gamma(N' + L' + \frac{3}{2}) (2L + 1)(2L' + 1)(2L_1 + 1)(2L_2 + 1)]^{1/2} \\ & \quad \times \sum_{L'_1 L'_2 L''_1 L''_2} (-1)^{L''_2} (2L'_1 + 1)(2L'_2 + 1)(2L''_1 + 1)(2L''_2 + 1) \begin{pmatrix} L'_1 & L'_2 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L''_1 & L''_2 & L' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L''_1 & L'_1 & L_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L''_2 & L'_2 & L_2 \\ 0 & 0 & 0 \end{pmatrix} \\ & \quad \times \sum_{JK} (2J + 1) \begin{pmatrix} L_1 & L_2 & J \\ M_1 & M_2 & K \end{pmatrix} \begin{pmatrix} L & L' & J \\ M & M' & K \end{pmatrix} \begin{Bmatrix} L'_1 & L'_2 & L \\ L''_1 & L''_2 & L' \\ L_1 & L_2 & J \end{Bmatrix} \\ & \quad \times \sum_{\nu_1 \nu_2} \sum_{\mu_1 \mu_2} \left(\frac{a}{a^2 + b^2} \right)^{L'_1 + L'_2 + 2(\nu_1 + \mu_2)} \left(\frac{b}{a^2 + b^2} \right)^{L''_1 + L''_2 + 2(\mu_1 + \nu_2)} \delta_{\nu_1 + \nu_2, N - P} \delta_{\mu_1 + \mu_2, N' - P} \\ & \quad \times \delta_{\nu_1 + \mu_1, N_1 - P_1} \delta_{\nu_2 + \mu_2, N_2 - P_2} [\nu_1! \nu_2! \mu_1! \mu_2! \Gamma(\nu_1 + L'_1 + \frac{3}{2}) \Gamma(\nu_2 + L'_2 + \frac{3}{2}) \\ & \quad \times \Gamma(\mu_1 + L''_1 + \frac{3}{2}) \Gamma(\mu_2 + L''_2 + \frac{3}{2})]^{-1} \end{aligned} \quad (A6)$$

in which

$$P = \frac{L'_1 + L'_2 - L}{2}, \quad P' = \frac{L''_1 + L''_2 - L'}{2}, \quad P_1 = \frac{L'_1 + L''_1 - L_1}{2}, \quad P_2 = \frac{L'_2 + L''_2 - L_2}{2}.$$

The energy, angular momentum, and parity conditions

$$\begin{aligned} 2N + L + 2N' + L' &= 2N_1 + L_1 + 2N_2 + L_2, \\ \mathbf{L} + \mathbf{L}' &= \mathbf{L}_1 + \mathbf{L}_2, \\ M + M' &= M_1 + M_2, \\ (-1)^{L + L'} &= (-1)^{L_1 + L_2}, \end{aligned} \quad (A7)$$

are contained in Eq. (A6), implicitly in the $3J$ symbols and explicitly in the delta functions.

In most cases we require the coupled brackets $\langle N_1 L_1, N_2 L_2 | N L, N' L'; J; a, b \rangle$ that occur in the coupled product expansion

$$[\Phi_{NL}(\mathbf{r}, B) \Phi_{N'L'}(\mathbf{r}', B)]_{JK} = \sum_{N_1 L_1} \sum_{N_2 L_2} \langle N_1 L_1, N_2 L_2 | N L, N' L'; J; a, b \rangle [\Phi_{N_1 L_1}(\mathbf{x}, B_1) \Phi_{N_2 L_2}(\mathbf{y}, B_2)]_{JK} \quad (A8)$$

and which are independent of the projection K . These are obtained from Eq. (A6) by dropping the sum on J and K and omitting the factor A where

$$A = (2J + 1) \begin{pmatrix} L_1 & L_2 & J \\ M_1 & M_2 & K \end{pmatrix} \begin{pmatrix} L & L' & J \\ M & M' & K \end{pmatrix}.$$

APPENDIX B: THE KERNEL $K(\mathbf{r}, \mathbf{r}')$

The kernel $K(\mathbf{r}, \mathbf{r}')$ is given in I as

$$\begin{aligned} K(\mathbf{r}, \mathbf{r}') &= \delta^3(\mathbf{r} - \mathbf{r}') + M(\mathbf{r}, \mathbf{r}') \langle STC | (36) | STC \rangle, \\ M(\mathbf{r}, \mathbf{r}') &= \frac{3^6 \sqrt{3}}{2^6} \frac{\beta^3}{\pi^{3/2}} e^{[-\beta^2 (15r^2/16 + 15r'^2/16 - (9/8)\mathbf{r} \cdot \mathbf{r}')]}, \end{aligned} \quad (B1)$$

where here we express $\langle STC | (36) | STC \rangle$ slightly differently from in I as

$$\langle STC | (36) | STC \rangle = \begin{cases} \frac{7}{27} & S = 0, T = 0 \\ -\frac{1}{81} & S = 1, T = 0 \text{ or } S = 0, T = 1 \\ \frac{31}{243} & S = 1, T = 1. \end{cases} \quad (B2)$$

Powers of K combine according to

$$\int d^3 r' K^\alpha(\mathbf{r}, \mathbf{r}') K^\beta(\mathbf{r}, \mathbf{r}') = \int d^3 r' K^{\alpha+\beta}(\mathbf{r}, \mathbf{r}'),$$

where $K^0(\mathbf{r}, \mathbf{r}') = \delta^3(\mathbf{r} - \mathbf{r}')$. Symbolically, we write $K^\alpha K^\beta = K^{\alpha+\beta}$.

To form K^{-1} or $K^{\pm 1/2}$ it is convenient to use a spectral representation. The eigenvalue problem for $K(\mathbf{r}, \mathbf{r}')$ is defined by

$$\int d^3 r' K(\mathbf{r}, \mathbf{r}') \eta_\alpha(\mathbf{r}') = \lambda_\alpha \eta_\alpha(\mathbf{r}). \quad (\text{B3})$$

We can equivalently solve

$$\int d^3 r' M(\mathbf{r}, \mathbf{r}') \eta_\alpha(\mathbf{r}') = \epsilon_\alpha \eta_\alpha(\mathbf{r}) \quad (\text{B4})$$

with

$$\lambda_\alpha = 1 + \epsilon_\alpha \langle STC | (36) | STC \rangle. \quad (\text{B5})$$

The problem posed in Eq. (B3) or (B4) is then of the general form

$$\int d^3 y e^{-(ax^2 + ay^2 - b\mathbf{x}\cdot\mathbf{y})} \eta_\alpha(\mathbf{y}) = E_\alpha \eta_\alpha(\mathbf{x}). \quad (\text{B6})$$

Since

$$e^{b\mathbf{x}\cdot\mathbf{y}} = \sum_{lm} I_l(bxy) Y_{lm}(\hat{x}) Y_{lm}^*(\hat{y}) \quad (\text{B7})$$

it is clear that $\eta_\alpha(\mathbf{x})$ has the form

$$\eta_\alpha(\mathbf{x}) \doteq F_{nl}(x) Y_{lm}(\hat{x}), \quad (\text{B8})$$

in which the set (nlm) now replaces α . When we substitute Eqs. (B7) and (B8) into Eq. (B6) and perform the angular integrations, we have the radial equation

$$\int y^2 dy e^{-ax^2} e^{-ay^2} F_{nl}(y) I_l(bxy) = E_{nl} F_{nl}(x). \quad (\text{B9})$$

Now

$$I_l(z) = 2\pi^{3/2} \sum_k \frac{(z/2)^{l+2k}}{k! \Gamma(l+k+\frac{3}{2})}. \quad (\text{B10})$$

So, for small x , $F_{nl}(x) \propto x^l$ whereas for large x , F_{nl} must fall as $\exp(-cx^2)$. Hence we write

$$F_{nl}(x) = x^l e^{-cx^2} G_{nl}(x). \quad (\text{B11})$$

When Eq. (B11) is inserted into Eq. (B9) and a power series expansion is made for $G_{nl}(x)$, one readily identifies G_{nl} as an associate Laguerre function⁵

$$G_{nl}(x) = L_n^{l+1/2}(2cx^2)$$

and

$$E_{nl} = (2\pi)^{3/2} b^l \frac{(2a-2c)^n}{(2a+2c)^{l+n+3/2}}$$

with

$$c = \left(a^2 - \frac{b^2}{4} \right)^{1/2}. \quad (\text{B12})$$

For our particular case $a = 15\beta^2/16$, $b = 9\beta^2/8$, so $c = 3\beta^2/4$. Also we find then

$$\epsilon_{nl} = -\left(\frac{1}{3}\right)^{l+2n-2}. \quad (\text{B13})$$

The normalized eigenfunctions of $M(\mathbf{r}, \mathbf{r}')$ are just isotropic harmonic oscillator radial functions $\phi_{nl}(\mathbf{r}, b)$ where the oscillator length parameter is given by

$$\beta b = \sqrt{\frac{2}{3}}. \quad (\text{B14})$$

Thus we finally have

$$\lambda_{nl} = 1 + \epsilon_{nl} \langle STC | (36) | STC \rangle \quad (\text{B15})$$

and

$$\int d^3 r' K(\mathbf{r}, \mathbf{r}') \Phi_{nlm}(\mathbf{r}', b) = \lambda_{nl} \Phi_{nlm}(\mathbf{r}, b). \quad (\text{B16})$$

For positive parity states $S = 1, T = 0$ or $S = 0, T = 1$ which requires l to be even. In that case, from Eq. (B2), $\langle STC | (36) | STC \rangle = -\frac{1}{81}$, so

$$\lambda_{nl} = 1 + \left(\frac{1}{3}\right)^{l+2n+2} \begin{cases} n = 0, 1, 2, \dots \\ l = 0, 2, 4, \dots \\ S = 1, T = 0; S = 0, T = 1. \end{cases}$$

For negative parity states, l is odd and $S = 0, T = 0$ or $S = 1, T = 1$. In the first case from Eq. (B2) it follows that

$$\lambda_{nl} = 1 - 7 \left(\frac{1}{3}\right)^{l+2n+1} \begin{cases} n = 0, 1, 2, \dots \\ l = 1, 3, 5, \dots \\ S = 0, T = 0, \end{cases}$$

while in the latter case

$$\lambda_{nl} = 1 - 31 \left(\frac{1}{3}\right)^{l+2n+3} \begin{cases} n = 0, 1, 2, \dots \\ l = 1, 3, 5, \dots \\ S = 1, T = 1. \end{cases}$$

In each case, λ_{nl} is clearly positive. Thus $K^{1/2}$ is defined and we may write

$$K^{-1/2}(\mathbf{r}, \mathbf{r}') = \delta^3(\mathbf{r} - \mathbf{r}') + \sum_{nlm} \bar{\lambda}_{nl} \Phi_{nlm}(\mathbf{r}, b) \Phi_{nlm}^*(\mathbf{r}', b) \quad (\text{B17})$$

where

$$\bar{\lambda}_{nl} = \lambda_{nl}^{-1/2} - 1. \quad (\text{B18})$$

The spectral representation of $K^{-1/2}(\mathbf{r}, \mathbf{r}')$ given by Eqs. (B16) and (B17) is used to form $K^{-1/2} H K^{-1/2}$ which we indicated was the matrix we diagonalize.

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