

The Theory of Hydrogen Three*†

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The binding energy of the triton has been calculated by the variational method. The forces between the particles are assumed to be charge independent and to be composed of central and tensor parts, the radial dependence of each being given by Yukawa wells. The binding energy calculation is employed to determine the range of the tensor component; the other constants are fixed by the low energy two-body data. The effective triplet range, the percentage D state in the triton, and the Coulomb energy of He^3 are then predicted. The first two of these are in satisfactory agreement with experiment; the third is in error by twenty-five percent. The final "best" potential contains only four constants, the ranges and depths of the central and tensor potentials. The triplet and singlet central forces are equal.

I. INTRODUCTION

IT is now well known that the low energy two-body data are not sensitive to the shape of the two-body nuclear potential. For this information it is more profitable to turn to high energy two-body scattering experiments and to the nuclear three-body system upon which our attention is focused here. This sensitivity of the three-body problem was recently discussed by Svartholm,¹ who employed several different central force potentials. We interpret his results as follows: If the range and depth of the internucleon potential are adjusted to the low energy two-body data, the calculated binding energy of H^3 will be greater for those wells which are deeper at small interparticle distances. Thus the Yukawa potential involving a $(1/r)$ singularity yields a larger binding energy than the Gaussian. This is in agreement with the calculation of Thomas,² who showed that the calculated binding energy of H^3 is infinite for a zero-range potential.

Svartholm also found that the calculated binding energy considerably exceeded the experimental value. We may take this as indirect evidence for the existence of noncentral forces (evidence of course not so cogent as is the existence of the quadrupole moment of the deuteron); for, as Inglis³ pointed out, such a force reduces the ratio of the theoretical H^3 binding energy to the binding energy of the deuteron.

In the present paper a variational calculation of the binding energy of H^3 and He^3 is made. The internucleon potential V_{12} between particles 1 and 2 is taken to be

$$V_{12} = -V_0 \left\{ \left[1 - \frac{1}{2}g + \frac{1}{2}g\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \right] f(r/r_c) + \gamma S_{12} f(r/r_t) \right\}, \quad (1)$$

where

$$S_{12} = r_{12}^{-2} [3(\boldsymbol{\sigma}_1 \cdot \mathbf{r}_{12})(\boldsymbol{\sigma}_2 \cdot \mathbf{r}_{12}) - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2],$$

$$f(x) = e^{-x}/x, \quad \mathbf{r}_{12} = \mathbf{r}_2 - \mathbf{r}_1,$$

and V_0 , γ , g , r_c , and r_t are constants. We assume charge independence of nuclear forces—which is consistent⁴ with the use of the Yukawa potential as far as low energy two-body data are concerned. Ideally the constants in potential (1) are fixed by the deuteron binding energy ϵ , the deuteron quadrupole moment Q , the singlet scattering length, the singlet effective range, and the triplet effective range ρ_1 . The singlet effective range is taken from p - p scattering data. The relation between these experimental results and the constants in our potential has been considered for the triplet state by Feshbach and Schwinger.⁵ The calculations of Hoisington, Share, and Breit⁶ and of Jackson and Blatt⁷ were employed in the determination of r_c and $V_0(1-2g)$, the only constants in the singlet potential; the numerical values are $r_c = 1.184 \times 10^{-13}$ cm, $V_0(1-2g) = 46.48$ Mev. At the time that these calculations were performed, the triplet effective range was not a very useful parameter. For a given tensor range r_t , ϵ and Q determine V_0 and γ quite closely. However, r_t itself is insensitive to ρ_1 , so that ρ_1 must be known very accurately before r_t is determined. As we shall see, the theoretical binding energy of H^3 is much more sensitive to r_t ; therefore, we employed it to determine r_t and then predicted ρ_1 . We obtain a rather close agreement with the most recent experimental values; hence we may conclude that potential (1) provides a good description of the nuclear two-body potential in the low energy domain.

Our results have a certain irreducible inaccuracy arising from, first, the possible existence of three-body forces⁸ and, second, the inaccuracy of potential (1) in the high energy domain.⁹ No corrections were made for these effects. If at some future time the two-body force is completely understood, the theory of H^3 will then be useful in the investigation of three-body forces.

We have also neglected exchange effects; however,

⁴ J. Schwinger, Phys. Rev. **78**, 135 (1950).

⁵ H. Feshbach and J. Schwinger, Phys. Rev. **84**, 194 (1951).

⁶ Hoisington, Share, and Breit, Phys. Rev. **56**, 884 (1939).

⁷ J. D. Jackson and J. M. Blatt, Revs. Modern Phys. **22**, 77 (1950).

⁸ H. Primakoff and T. Holstein, Phys. Rev. **55**, 1218 (1939).

⁹ R. S. Christian and E. W. Hart, Phys. Rev. **77**, 441 (1950); R. S. Christian and H. P. Noyes, Phys. Rev. **79**, 85 (1950).

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† A preliminary report was published as a Letter to the Editor, Phys. Rev. **81**, 142 (1951).

‡ Now at the RAND Corporation, Santa Monica, California.

¹ N. Svartholm, thesis, Lund (H. Ohlssons Boktryckeri, 1945).

² L. H. Thomas, Phys. Rev. **47**, 903 (1935).

³ D. R. Inglis, Phys. Rev. **55**, 988 (1939).

both Svartholm¹ and Hu and Hsu¹⁰ have found that these have very little effect.

Other calculations which have been made with tensor forces include those of Gerjuoy and Schwinger,¹¹ Feshbach and Rarita,¹² and Clapp.¹³ These authors employed the Rarita-Schwinger potential,¹⁴ which is, however, no longer in agreement with experiment. Hu and Hsu¹⁰ have made calculations employing a potential of form (1), but primarily with $r_c=r_t$, the values of r_c chosen precluding any charge independence. A preliminary calculation in which $r_c \neq r_t$ was made by Avery and Adams.¹⁵

II. VARIATIONAL PROCEDURE

The major portion of the investigation consisted in constructing a nuclear Hamiltonian with potentials given by (1), choosing suitable trial wave functions, and determining an upper bound to the ground-state energy by means of the Ritz variation method.

Choice of the relative coordinate system of Fig. 1 permitted the expression of the D state wave functions in terms of operations upon the S state wave functions by operators of the form S_{ij} . In such a system, the kinetic energy

$$T = -\frac{\hbar^2}{M}(\nabla_1^2 + \nabla_1 \cdot \nabla_2 + \nabla_2^2), \quad (2)$$

where M is the nucleon mass.

The trial functions were chosen to be combinations of the spin-antisymmetric ${}^2S_{\frac{1}{2}}$ state and the three independent ${}^4D_{\frac{3}{2}}$ states, designated, respectively, D , D' , and D'' . The other possible ${}^2S_{\frac{1}{2}}$ state, symmetric in the neutron spins and thus antisymmetric in the neutron space coordinates, was not used because it vanished for $r_1=r_2$; Feshbach and Rarita¹² found that it added only 0.4 percent to their computed binding energy. Since the S - P coupling was of higher order than the S - D coupling and the percentage D state was less than 4 percent, no P states were included. The four spin-

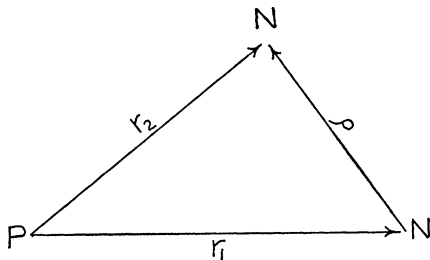


FIG. 1. Coordinate system for H^3 .

TABLE I. Comparison of results. The entries in columns labeled Step 1, Step 2, and Step 5 are the respective calculated binding energies in Mev for the four-term wave function (Step 1), the five-term wave function (Step 2), and the nine-term wave function (Step 5). The units of r_t are 10^{-13} cm.

r_t	r_t/r_c	Step 1	Step 2	Step 5
2.122	1.792	-9.10	-9.46	-10.05
1.827	1.543	-7.86	-8.21	-9.06
1.533	1.294	-5.72	-6.06	-7.50

angular wave functions were

$$\begin{aligned} \chi_S &= (2)^{-3}[\alpha(1)\beta(2) - \beta(1)\alpha(2)]\alpha(3), \\ \chi_D &= [r_1^2 S_{13} + r_2^2 S_{23}]\chi_S, \\ \chi_{D'} &= [r_1^2 S_{13} - r_2^2 S_{23}]\chi_S, \\ \chi_{D''} &= [3(\sigma_1 \cdot \mathbf{r}_1 \times \mathbf{r}_2)(\sigma_3 \cdot \mathbf{r}_1 \times \mathbf{r}_2) \\ &\quad - (\sigma_1 \cdot \sigma_3)(\mathbf{r}_1 \times \mathbf{r}_2) \cdot (\mathbf{r}_1 \times \mathbf{r}_2)]\chi_S. \end{aligned} \quad (3)$$

If the trial wave function is $\sum |i\rangle A_i$, then the Ritz variation method automatically chooses optimum values of A_i through solution of the secular determinant

$$|(i|H-E|j)| = 0, \quad (4)$$

where $|i\rangle$ and $|j\rangle$ represent typical terms. For convenience in computation, the matrix elements were broken up into a sum of terms:

$$\begin{aligned} (i|H-E|j) &= \frac{\hbar^2}{M}(i|KE|j) + (i|V|j)_{NT} \\ &\quad + 2(i|T_{13}|j) + (i|T_{12}|j) - E(i|j). \end{aligned} \quad (5)$$

The sign of the "KE" matrix element was changed for convenience. The "NT" (nontensor) elements arise from the central-force potential terms and are grouped together because of similarity. The three matrix elements of the tensor-force part of the potential, involving S_{13} , S_{23} , and S_{12} , respectively, were designated as $(i|T_{13}|j)$, $(i|T_{23}|j)$, and $(i|T_{12}|j)$, the first two of which are equal. After summation over spins, spatial integration was carried out by the techniques of Hylleraas¹⁶ and of Coolidge and James.^{16,17}

The variational calculation began with a four-term trial function and proceeded to a more complex trial function in a series of stages:

† *Step 1.* A four-term trial function was used, with one term for each spin state, of the form

$$\begin{aligned} \psi^{(1)} &= A_S \psi_S + A_D \psi_D + A_{D'} \psi_{D'} + A_{D''} \psi_{D''}, \\ \psi_S &= \chi_S \exp -\frac{1}{2}\lambda(r_1 + r_2 + \rho), \\ \psi_D &= \chi_D \exp -\frac{1}{2}\mu(r_1 + r_2 + \rho), \\ \psi_{D'} &= \chi_{D'}(r_1 - r_2) \exp -\frac{1}{2}\nu(r_1 + r_2 + \rho), \\ \psi_{D''} &= \chi_{D''}(r_1 - r_2) \exp -\frac{1}{2}\omega(r_1 + r_2 + \rho). \end{aligned} \quad (6)$$

Reasonable values for λ , μ , and ν were determined by applying the Ritz method to the first three terms. Then

¹⁶ E. A. Hylleraas, *Z. Physik* **54**, 347 (1929); A. S. Coolidge and H. M. James, *Phys. Rev.* **51**, 855 (1937).

¹⁷ See Appendix A.

¹⁰ T.-M. Hu and K.-N. Hsu, *Phys. Rev.* **78**, 633 (1950).

¹¹ E. Gerjuoy and J. Schwinger, *Phys. Rev.* **61**, 138 (1942).

¹² H. Feshbach and W. Rarita, *Phys. Rev.* **75**, 1384 (1949).

¹³ R. E. Clapp, *Phys. Rev.* **76**, 873 (1949).

¹⁴ W. Rarita and J. Schwinger, *Phys. Rev.* **59**, 436 (1941).

¹⁵ R. Avery and E. N. Adams, *Phys. Rev.* **75**, 1106 (1949).

TABLE II. Physical results.^a

r_t	r_t/r_c	E	γ	V_0	g	P_D	E_{Coul}	ρ_1
2.122	1.792	-10.05	0.2259	55.054	0.0779	2.2	1.088	1.79
1.827	1.543	-9.06	0.3799	50.123	0.0364	2.8	1.059	1.76
1.70	1.44	-8.48 ^b	0.5085	46.96	0.005	3.1	1.041	1.74
1.56	1.32	-7.63 ^c	0.7365	42.00	-0.053	3.5	1.014	1.72
1.533	1.294	-7.50	0.7894	40.918	-0.0679	3.6	1.008 _s	1.71

^a Unit of length 10^{-13} cm; unit of energy 1 Mev.

^b Experimental value of binding energy.

^c 90 percent of experimental value of binding energy.

the fourth term was added and E was minimized for ω ; it was found that the inclusion of the D'' term contributed about 5 percent to the computed energy. Next, the 4×4 determinant was minimized in E simultaneously for λ , μ , and ν , using the value of ω previously determined. Finally, ω was varied slightly. Incidentally, we would like to note that ψ_S is an exceedingly good trial function for the pure central force case. When employed with the exponential or Yukawa wells it gives well over 90 percent of the binding energy obtained by Rarita and Present¹⁸ and Svartholm,¹ respectively.

Step 2. A five-term trial function was formed by increasing the number of S terms to two. The S part of the wave function had the form

$$A_{S1}\psi_{S1} + A_{S2}\psi_{S2}, \quad (7)$$

$$\psi_{Si} = \chi_S \exp[-\frac{1}{2}\lambda_i(r_1+r_2+\rho)].$$

The energy was minimized for variation of the five parameters λ_1 , λ_2 , μ , ν , and ω .

Step 3. A seven-term trial function (S_1 , S_2 , D_1 , D_2 , D_1' , D_2' , D'') was formed from the function of Step 2 by splitting the D and D' states, just as was done in Step 2 to the S states. The parameters λ_1 , λ_2 , and ω were retained from Step 2, and the energy was minimized for variations of the four parameters μ_1 , μ_2 , ν_1 , and ν_2 .

Step 4. The wave function of Step 2 was enlarged by multiplying the S terms by series in $(r_1-r_2)^2$, in ρ , and in (r_1+r_2) ; i.e., such that the S parts of the wave function assumed such forms as

$$[A_{S1} + A_{S1}^*(r_1-r_2)^2] \exp[-\frac{1}{2}\lambda_1(r_1+r_2+\rho)] + (S_1 \rightleftharpoons S_2),$$

$$[A_{S1} + A_{S1}^*\rho] \exp[-\frac{1}{2}\lambda_1(r_1+r_2+\rho)] + (S_1 \rightleftharpoons S_2),$$

$$[A_{S1} + A_{S1}^*(r_1+r_2)] \exp[-\frac{1}{2}\lambda_1(r_1+r_2+\rho)] + (S_1 \rightleftharpoons S_2),$$

where the symbol $(S_1 \rightleftharpoons S_2)$ denotes a similar expression

involving the S_2 term. The five parameters λ_1 , λ_2 , μ , ν , and ω were retained from Step 2.

Step 5. A procedure similar to that of Step 4 was applied to the D and D' states. A series involving ρ , a series involving (r_1+r_2) , and then a series involving both were used.

Steps 3 and 4 did not produce a sufficient decrease in computed energy to justify the correspondingly increased complexity of the wave function, and hence were dropped. However, Step 5 was retained; the final wave function was

$$\psi = A_{S1}\psi_{S1} + A_{S2}\psi_{S2} + [A_D + \rho A_{D^*} + (r_1+r_2)A_{D^0}]\psi_D$$

$$+ [A_{D'} + \rho A_{D'^*} + (r_1+r_2)A_{D'^0}]\psi_{D'} + A_{D''}\psi_{D''}. \quad (8)$$

The behavior of the calculated binding energy as the wave function was improved is shown in Table I. For tensor ranges $r_t = 2.122 \times 10^{-13}$ cm and 1.827×10^{-13} cm (corresponding, respectively, to $r_t/r_c = 1.792$ and 1.543), convergence seems to have been obtained. The results for $r_t = 1.533 \times 10^{-13}$ cm ($r_t/r_c = 1.294$) are somewhat more uncertain, but we estimate the computed binding energy to be no more than a few percent above the correct value.

III. RESULTS

Matrix elements obtained after removal of spin dependence are tabulated in Appendix B.¹⁹

Table II shows the constants of the assumed inter-nuclear potential (1), both for the three values of r_t for which the calculations were carried through and (by interpolation) for cases corresponding to variationally computed energies of 7.63 and 8.48 Mev, which represent, respectively, 90 percent and 100 percent of the experimental value.²⁰ Calculated percent D state, Coulomb energy, and effective triplet scattering ranges for the above cases are also shown. Wave function parameters are shown in Table III.

IV. DISCUSSION

Inspection of Table II reveals the sensitivity of the computed triton binding energy to variations in the range of the tensor force; the computation of triton binding energy thus allows a sharply defined tensor range to be set. One can see that the triplet effective range is not nearly so sensitive to variations in tensor range as the binding energy is.

However, the above does not necessarily indicate that a large effect upon the properties of the system is

TABLE III. Wave function parameters.

r_t/r_c	$\lambda_1 r_c$	$\lambda_2 r_c$	μr_c	νr_c	ωr_c	A_{S1}	A_{S2}	A_D	$A_{D'}$	$A_{D''}$	A_{D^*}	$A_{D'^*}$	A_{D^0}	$A_{D'^0}$
• 1.792	1.0	2.0	2.2	2.5	2.8	1.464	4.672	1.0	-1.204	0.693	0.426	-0.1085	-0.248	0.168
• 1.543	1.0	1.9	2.2	2.5	2.8	1.369	3.537	1.0	-1.178	0.902	0.493	-0.1945	-0.269	0.180
1.44	0.9 ₅	1.8	2.2	2.5	2.8	1.08	3.01	1.0	-1.29	0.91	0.45	-0.136	-0.27	0.20
1.32	0.8	1.5 ₅	2.2	2.5	2.8	0.44	2.36	1.0	-1.59	0.80	0.30	0.058	-0.25	0.25
• 1.294	0.8	1.5	2.2	2.5	2.8	0.272	2.241	1.0	-1.666	0.758	0.254	0.1129	-0.241	0.263

¹⁸ W. Rarita and R. D. Present, Phys. Rev. **51**, 788 (1937).

¹⁹ Integrated matrix elements are not shown because of space limitations, but are available in hectographed form.

²⁰ Li, Whaling, Fowler, and Lauritsen, Phys. Rev. **83**, 512 (1951).

produced by variations of r_i alone, for the requirement that two-body data be satisfied necessitates a change in γ , V_0 , and g when r_i is changed, and r_i occurs in the expression for tensor well depth as well.

From Table II, we see that the appropriate value of r_i is 1.70×10^{-13} cm. The corresponding value of ρ_1 is 1.74×10^{-13} cm. This agrees very well with the experimental value²¹ of 1.71×10^{-13} cm. The corresponding value of the percent D state is 3.1 percent, which is to be compared with the value 3.7₅ percent obtained by the theory of Sachs and Schwinger²² from the sum of the magnetic moments of H^3 and He^3 . This agreement seems satisfactory, in view of the uncertainties arising from relativistic effects in the Sachs and Schwinger calculation. We finally turn to the Coulomb energy, the expectation value of e^2/ρ , equal to the difference in H^3 and He^3 binding energies. The predicted Coulomb energy is higher than the experimental value of 0.77 Mev.²³ This discrepancy may be in part due to the unsuitability for this calculation of our wave function, determined as it has been by a variational expression for the energy. Further explanations of the discrepancy include the following possibilities: (1) effects of the magnetic interaction; (2) inequality of $n-p$ and $\bar{p}-\bar{p}$ forces; (3) requirement that the potential be less singular at zero interparticle distances than is the Yukawa potential. The first of these has been investigated.²⁴ It is found that the magnetic effects increase the binding energy difference between H^3 and He^3 ; thus the discrepancy is increased. Suggestion (2) can hardly be investigated at the present time. Meson field theory does, however, indicate that higher order effects of this kind do exist. Suggestion (3) is buttressed to some extent by the fact⁹ that the exponential well does give a better value for the total $n-p$ cross section at high energy than the Yukawa well. On the other hand, the latter yields a better angular distribution.

In conclusion, potential (1) with the constants given in Table II for $E = -8.48$ Mev summarizes all the low energy two-body data and gives the correct binding energy and percent D state for H^3 . A discrepancy of twenty-five percent in the Coulomb energy remains.

Note that by only a slight reduction of the range of the tensor forces one may place g equal to zero, for which the singlet and triplet central potentials are equal. This four-parameter potential is consistent with the experimental data and is more satisfying in that these four constants predict six experimental numbers, the singlet and triplet scattering lengths and effective ranges, the deuteron quadrupole moment, and the binding energy of H^3 .²⁵

²¹ Hughes, Burgy, and Ringo, Phys. Rev. **77**, 291 (1950).

²² R. G. Sachs and J. Schwinger, Phys. Rev. **70**, 41 (1946).

²³ Tollestrup, Jenkins, Fowler, and Lauritsen, Phys. Rev. **75**, 1947 (1949).

²⁴ George Stuart (private communication).

²⁵ Note added in proof: Recent calculations by Irving [Phys. Rev. **87**, 519 (1952)] indicate that this potential will also predict the binding energy of He^4 with fair accuracy.

We are greatly indebted to Dr. Jane S. Pease for verifying some of our calculations. Most of the numerical work was ably and patiently performed by Miss Hannah Paul of the Joint Computing Group at the Massachusetts Institute of Technology.

APPENDIX

A. Methods of Integration

Since the Hamiltonian is independent of the location or orientation of the system, the only noncyclic coordinates are r_1, r_2 , and ρ or a system derived from them. The general volume element may be shown rigorously by direct computation of the Jacobian to be

$$(8/3)\pi^2 r_1 r_2 \rho dr_1 dr_2 d\rho;$$

we can, however, drop the numerical factor for simplicity.

The integration limits on the above set of variables involve, for the first variable integrated, the sum and (absolute value of) the difference of the other two variables. As this is rather unwieldy where exponentials are involved, we shall use two other schemes in actual computations.

Integration of the matrix elements involving exponentially only (r_1+r_2) and ρ is carried out most simply by the Hylleraas method as used by Rarita and Present.¹⁸ If one chooses as variables the quantities $s \equiv r_1+r_2$, $t \equiv r_1-r_2$, and ρ , the integration scheme becomes

$$\int f(s, t, \rho) d\tau = \int_0^\infty ds \int_0^s d\rho \int_0^\rho dt \rho (s^2 - t^2) f(s, t, \rho), \quad (A1)$$

for which recursion formulas were developed.¹⁸

However, this scheme proved overly difficult where the exponentials involved r_1 and r_2 unsymmetrically. Instead of permuting the variables, we used the scheme of Coolidge and James,¹⁶ which has the advantage of compartmenting the integrations. Making the substitutions

$$\begin{aligned} \xi &\equiv r_1 + r_2 - \rho, \\ \eta &\equiv r_1 - r_2 + \rho, \\ \zeta &\equiv -r_1 + r_2 + \rho, \end{aligned} \quad (A2)$$

and inserting a numerical factor chosen simply to give the same result as the Hylleraas method for the same integrand, one obtains

$$\begin{aligned} \int f(\xi, \eta, \zeta) d\tau &= (1/8) \int_0^\infty d\xi \int_0^\infty d\eta \int_0^\infty d\zeta \\ &\times (\xi + \eta)(\xi + \zeta)(\eta + \zeta) f(\xi, \eta, \zeta). \end{aligned} \quad (A3)$$

When $(\xi + \eta)^3$ appears in the denominator of $f(\xi, \eta, \zeta)$, the integration cannot be carried out independently over ξ and η , but the integrals may easily be evaluated

by the further substitutions

$$\xi = y - x, \quad \eta = y + x, \quad (\text{A4})$$

or the substitutions

$$\xi = r \cos^2 \phi, \quad \eta = r \sin^2 \phi. \quad (\text{A5})$$

B. Matrix Elements, Not Integrated

Let typical S , D , D' , and D'' components of the trial wave function be, respectively, $b(r_1, r_2, \rho)\chi_S$, $g(r_1, r_2, \rho)\chi_D$, $h(r_1, r_2, \rho)\chi_{D'}$, and $p(r_1, r_2, \rho)\chi_{D''}$. Then the matrix elements, expressed as integrals over spatial coordinates, are as follows:

1. Normalization Elements

$$(S|S) = \int b^2 d\tau$$

$$(S|D) = 0$$

$$(S|D') = 0$$

$$(S|D'') = 0$$

$$(D|D) = \int g^2 d\tau 6[r_1^4 + r_2^4 + r_1^2 r_2^2 (1 - 3 \cos^2 \theta)]$$

$$(D|D') = \int gh d\tau 6[r_1^4 - r_2^4]$$

$$(D|D'') = \int gp d\tau (-3)(r_1^2 - r_2^2)r_1^2 r_2^2 (1 - \cos^2 \theta)$$

$$(D'|D') = \int h^2 d\tau 6[r_1^4 + r_2^4 - r_1^2 r_2^2 (1 - 3 \cos^2 \theta)]$$

$$(D'|D'') = \int hp d\tau (-3)(r_1^2 + r_2^2)r_1^2 r_2^2 (1 - \cos^2 \theta)$$

$$(D''|D'') = \int p^2 d\tau 6[r_1^2 r_2^2 (1 - \cos^2 \theta)]^2$$

$$\cos \theta = (r_1^2 + r_2^2 - \rho^2) / 2r_1 r_2.$$

2. Kinetic Energy Elements

Let

$$\begin{aligned} P(u, v) \equiv & \frac{u}{r_1^2} \frac{\partial}{\partial r_1} \left(r_1^2 \frac{\partial v}{\partial r_1} \right) + \frac{u}{r_2^2} \frac{\partial}{\partial r_2} \left(r_2^2 \frac{\partial v}{\partial r_2} \right) \\ & + \frac{u}{\rho^2} \frac{\partial}{\partial \rho} \left(\rho^2 \frac{\partial v}{\partial \rho} \right) + \frac{\mathbf{r}_1 \cdot \mathbf{r}_2}{r_1 r_2} u \frac{\partial^2 v}{\partial r_1 \partial r_2} \\ & - \frac{\mathbf{r}_1 \cdot \boldsymbol{\rho}}{r_1 \rho} u \frac{\partial^2 v}{\partial r_1 \partial \rho} + \frac{\mathbf{r}_2 \cdot \boldsymbol{\rho}}{r_2 \rho} u \frac{\partial^2 v}{\partial r_2 \partial \rho}. \end{aligned}$$

Then

$$(S|KE|S) = - \int d\tau P(b, b)$$

$$(S|KE|D) = 0$$

$$(S|KE|D') = 0$$

$$(S|KE|D'') = 0$$

$$\begin{aligned} (D|KE|D) = & - \int d\tau \left\{ \left[P(g, g) + \frac{2g}{\rho} \frac{\partial g}{\partial \rho} \right] \right. \\ & \times 6[r_1^4 + r_2^4 + r_1^2 r_2^2 (1 - 3 \cos^2 \theta)] + \frac{4g}{r_1} \frac{\partial g}{\partial r_1} \\ & \times [6r_1^4 + 3r_1^2 r_2^2 (1 - 3 \cos^2 \theta) - 3(r_1^2 - r_2^2)r_1 r_2 \cos \theta] \\ & \left. + \frac{4g}{r_2} \frac{\partial g}{\partial r_2} [6r_2^4 + 3r_1^2 r_2^2 (1 - 3 \cos^2 \theta) \right. \\ & \left. + 3(r_1^2 - r_2^2)r_1 r_2 \cos \theta] \right\} \end{aligned}$$

$$\begin{aligned} (D|KE|D') = & - \int d\tau \left\{ \left[P(g, h) 6(r_1^4 - r_2^4) + \frac{4g}{r_1} \frac{\partial h}{\partial r_1} \right] \right. \\ & \times [6r_1^4 + 3r_1^2 r_2^2 (1 - 3 \cos^2 \theta) + 3(r_1^2 - r_2^2)r_1 r_2 \cos \theta] \\ & + \frac{4g}{r_2} \frac{\partial h}{\partial r_2} [-6r_2^4 - 3r_1^2 r_2^2 (1 - 3 \cos^2 \theta) \\ & \left. + 3(r_1^2 - r_2^2)r_1 r_2 \cos \theta] + \frac{4g}{\rho} \frac{\partial h}{\partial \rho} [3(r_1^4 - r_2^4) \right. \\ & \left. - 6(r_1^2 - r_2^2)r_1 r_2 \cos \theta] \right\} \end{aligned}$$

$$\begin{aligned} (D|KE|D'') = & - \int d\tau \left\{ \left[P(g, p) + \frac{4g}{r_1} \frac{\partial p}{\partial r_1} + \frac{4g}{r_2} \frac{\partial p}{\partial r_2} \right. \right. \\ & \left. \left. + \frac{4g}{\rho} \frac{\partial p}{\partial \rho} \right] (-3)(r_1^2 - r_2^2)r_1^2 r_2^2 (1 - \cos^2 \theta) \right. \\ & \left. + gp [-12(r_1^4 - r_2^4) + 12(r_1^2 - r_2^2)r_1 r_2 \cos \theta] \right\} \end{aligned}$$

$$\begin{aligned} (D'|KE|D') = & - \int d\tau \left\{ [P(h, h)] \right. \\ & \times 6[r_1^4 + r_2^4 - r_1^2 r_2^2 (1 - 3 \cos^2 \theta)] + \frac{4h}{r_1} \frac{\partial h}{\partial r_1} \\ & \times [6r_1^4 - 3r_1^2 r_2^2 (1 - 3 \cos^2 \theta) + 3(r_1^2 + r_2^2)r_1 r_2 \cos \theta] \\ & + \frac{4h}{r_2} \frac{\partial h}{\partial r_2} [6r_2^4 - 3r_1^2 r_2^2 (1 - 3 \cos^2 \theta) \\ & \left. + 3(r_1^2 + r_2^2)r_1 r_2 \cos \theta] + \frac{4h}{\rho} \frac{\partial h}{\partial \rho} [3(r_1^4 + r_2^4) \right. \\ & \left. - 3r_1^2 r_2^2 (1 - 3 \cos^2 \theta) - 6(r_1^2 + r_2^2)r_1 r_2 \cos \theta] \right\} \end{aligned}$$

$$(D'|KE|D'') = - \int d\tau \left\{ \left[P(h, p) + \frac{4h}{r_1} \frac{\partial p}{\partial r_1} + \frac{4h}{r_2} \frac{\partial p}{\partial r_2} + \frac{4h}{\rho} \frac{\partial p}{\partial \rho} \right] (-3)(r_1^2 + r_2^2)r_1^2 r_2^2 (1 - \cos^2 \theta) + hp[-12(r_1^4 + r_2^4) - 12r_1^2 r_2^2 (1 - 3 \cos^2 \theta) + 12(r_1^2 + r_2^2)r_1 r_2 \cos \theta] \right\}$$

$$(D''|KE|D'') = - \int d\tau \left\{ \left[P(p, p) + \frac{4p}{r_1} \frac{\partial p}{\partial r_1} + \frac{4p}{r_2} \frac{\partial p}{\partial r_2} + \frac{4p}{\rho} \frac{\partial p}{\partial \rho} \right] [6[r_1^2 r_2^2 (1 - \cos^2 \theta)]^2 + p^2 [6(r_1^2 + r_2^2 - r_1 r_2 \cos \theta)r_1^2 r_2^2 (1 - \cos^2 \theta)]] \right\}.$$

3. Nontensor Potential Elements

$$(S|V|S)_{NT} = -V_0 \int b^2 d\tau \times \left\{ (1 - \frac{1}{2}g)[f(r_1/r_c) + f(r_2/r_c)] + (1 - 2g)f(\rho/r_c) \right\}.$$

With the exception of the $S-S$ element, the nontensor potential elements are the same as the corresponding normalization elements, premultiplied by $(-V_0)$, and with a factor of

$$[f(r_1/r_c) + f(r_2/r_c) + f(\rho/r_c)].$$

inserted into the integrand. As a typical example,

$$(D|V|D')_{NT} = -V_0 \int gh d\tau 6(r_1^4 - r_2^4) \times [f(r_1/r_c) + f(r_2/r_c) + f(\rho/r_c)].$$

4. T_{13} Potential Elements

$$(S|T_{13}|S) = 0$$

$$(S|T_{13}|D) = -\gamma V_0 \int bg d\tau f(r_1/r_i) \times [6r_1^2 + (3 - 9 \cos^2 \theta)r_2^2]$$

$$(S|T_{13}|D') = -\gamma V_0 \int bhd\tau f(r_1/r_i) \times [6r_1^2 - (3 - 9 \cos^2 \theta)r_2^2]$$

$$(S|T_{13}|D'') = +\gamma V_0 \int bpd\tau f(r_1/r_i) [3r_1^2 r_2^2 (1 - \cos^2 \theta)]$$

$$(D|T_{13}|D) = -\gamma V_0 \int g^2 d\tau f(r_1/r_i) \times [-12r_1^4 + 6(r_2^4 - 2r_1^2 r_2^2)(1 - 3 \cos^2 \theta)]$$

$$(D|T_{13}|D') = -\gamma V_0 \int gh d\tau f(r_1/r_i) \times [-12r_1^4 - 6r_2^4(1 - 3 \cos^2 \theta)]$$

$$(D|T_{13}|D'') = -\gamma V_0 \int gpd\tau f(r_1/r_i) [6r_1^4 r_2^2 (1 - \cos^2 \theta) + 3r_1^2 r_2^4 (4 - 10 \cos^2 \theta + 6 \cos^4 \theta)]$$

$$(D'|T_{13}|D') = -\gamma V_0 \int h^2 d\tau f(r_1/r_i) [-12r_1^4 + 6r_2^4(1 - 3 \cos^2 \theta) + 12r_1^2 r_2^2 (1 - 3 \cos^2 \theta)]$$

$$(D''|T_{13}|D'') = -\gamma V_0 \int hpd\tau f(r_1/r_i) [6r_1^4 r_2^2 (1 - \cos^2 \theta) - 3r_1^2 r_2^4 (4 - 10 \cos^2 \theta + 6 \cos^4 \theta)]$$

$$(D''|T_{13}|D'') = -\gamma V_0 \int p^2 d\tau f(r_1/r_i) 6[r_1^2 r_2^2 (1 - \cos^2 \theta)]^2.$$

5. T_{12} Potential Elements

$$(S|T_{12}|S) = 0$$

$$(S|T_{12}|D) = 0$$

$$(S|T_{12}|D') = 0$$

$$(S|T_{12}|D'') = 0$$

$$(D|T_{12}|D) = -\gamma V_0 \int g^2 d\tau f(\rho/r_i)$$

$$\times \left\{ 12[r_1^4 + r_2^4 + \frac{1}{2}r_1^2 r_2^2 (3 \cos^2 \theta - 1)] \right.$$

$$\left. - \frac{12}{\rho^2} [2r_1^6 + 2r_2^6 + r_1^2 r_2^2 (r_1^2 + r_2^2) \right.$$

$$\left. + (2r_1^2 r_2^2 - 4r_1^4 - 4r_2^4)r_1 r_2 \cos \theta \right\}$$

$$(D|T_{12}|D') = -\gamma V_0 \int gh d\tau f(\rho/r_i) \left\{ 12(r_1^4 - r_2^4) \right.$$

$$\left. - \frac{12}{\rho^2} [2r_1^6 - 2r_2^6 + \frac{1}{2}r_1^2 r_2^2 (r_1^2 - r_2^2) \right.$$

$$\left. - 4(r_1^4 - r_2^4)r_1 r_2 \cos \theta + \frac{3}{2}(r_1^2 - r_2^2)r_1^2 r_2^2 \cos^2 \theta \right\}$$

$$(D|T_{12}|D'') = -\gamma V_0 \int gpd\tau f(\rho/r_i)$$

$$\times 6(r_1^2 - r_2^2)r_1^2 r_2^2 (1 - \cos^2 \theta)$$

$$(D'|T_{12}|D') = -\gamma V_0 \int h^2 d\tau f(\rho/r_i) \left\{ 12[r_1^4 + r_2^4 \right.$$

$$\left. + \frac{1}{2}r_1^2 r_2^2 (1 - 3 \cos^2 \theta) \right] - \frac{12}{\rho^2} [2r_1^6 + 2r_2^6$$

$$- 2(2r_1^4 + r_1^2 r_2^2 + 2r_2^4)r_1 r_2 \cos \theta$$

$$\left. + 3(r_1^2 + r_2^2)r_1^2 r_2^2 \cos^2 \theta \right\}$$

$$(D''|T_{12}|D'') = -\gamma V_0 \int hpd\tau f(\rho/r_i)$$

$$\times \left\{ 6(r_1^2 + r_2^2)r_1^2 r_2^2 (1 - \cos^2 \theta) - \frac{36}{\rho^2} [r_1^2 r_2^2 (1 - \cos^2 \theta)]^2 \right\}$$

$$(D''|T_{12}|D'') = -\gamma V_0 \int p^2 d\tau f(\rho/r_i) 6[r_1^2 r_2^2 (1 - \cos^2 \theta)]^2.$$