REALISTIC SOFT-CORE POTENTIALS
IN THE
BOUND THREE-NUCLEON SYSTEM

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SCOPE AND CONTENTS:

Variational calculations of the bound three-nucleon system have been done. Gaussian type trial functions were chosen which led to an explicit decomposition of the three-body wave function into components which display definite two-body LSJ dependence. The calculations were done with three soft-core potentials and one purely attractive potential. It was found that regardless of the number of terms the superposition of Gaussians was inferior to exponential trial functions. A correction in the binding for the Gaussian type function was applied and it was found that the modern realistic soft-core potentials are not inconsistent with the experimentally observed binding of the triton. The Coester-Yen potential, although it is "unrealistic", gives binding energy and radius of the triton which are in close agreement with experiment.

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CHAPTER I

INTRODUCTION

Over the past decade or so a great deal of effort has been expended on local repulsive-core nucleon-nucleon potentials which fit a wide range of two-body data. Such repulsive-core potentials are treated in a straightforward manner in the two-body system, but lead to considerable complications in the three- and four-body nuclei. Recently very accurate calculations on the triton have been done using purely central forces with a hard core (TSH65; RB66). To date only Blatt et al. have calculated the triton binding energy with realistic repulsive-core forces (DMB61; BDL62; BD64; DB67; D67). Blatt and Delves (DB67) have done the calculation for the Gammel-Thaler, Hamada-Johnston, and Yale potentials. All these potentials contain hard cores, central, non-central tensor, and $\vec{L}\cdot\vec{S}$ components. The Hamada-Johnston and Yale potentials have additional quadratic $\vec{L}\cdot\vec{S}$ components. Table I-1 lists the results of the most recent calculations. In Table I-2 we have given the experimentally determined quantities that one tries to predict in the triton calculations.

Whereas the most recent calculations are of a variational nature and are quite general, a modification to that approach is required in order to treat the more recent realistic potentials, such as the Reid soft-core (R68) and the Kerman-Bressel potentials (BKR68). The reason for a different approach lies in the functional behaviour of the recent potentials. Blatt *et al*. had to deal with infinite repulsive cores in the potentials that they used. They did this by making their trial function zero inside and at the boundary of the infinitely repulsive force region; thus ensuring zero probability that two particles come closer to each other than the core radius. The Reid and Kerman-Bressel potentials, however, have "soft" repulsive cores. The short range behaviour of the nucleons is described by strong but finite repulsion. This means that the wave function does not vanish although its amplitude becomes very small in the repulsive force region. In a calculation with soft core potentials, one must ensure that the wave function behaves in this way.

Since the potentials used by Blatt *et al*. are expressed as a sum of central, tensor, spin-orbit, and quadratic spin-orbit forces, they can also be expressed in terms of the spin and parity state of the two interacting particles. In order to calculate the potential energy matrix elements, they use this feature (D60). The Reid potential, however, is given separately for each LSJ state. It is difficult to project from Blatt *et al*.'s trial functions such LSJ dependence. For this reason also an alternative approach is required.

Soft-Core Potentials

Since fairly accurately fitted realistic soft-core potentials have recently become available, it is of interest to look at their effect in nuclear structure. The calculations of binding energy per particle in nuclear matter seem to indicate that potentials with infinitely hard repulsive cores give too little binding (BM62; R63). The static soft-core potential used by C. Wong (W65) acting only in the $^1S_0$ state was estimated to give more binding in nuclear matter than the hard-core potential. The same conclusion was reached by Bhargava and Sprung (BS67) when they compared the results of the Hamada-Johnston and Reid hard-core potentials with that of the soft-core Bressel-Kerman potential. Recently Sprung (S68) compared the effect of the Reid hard-core with the effect of Reid soft-core (R68). He found that the soft-core potential gave about 3MeV more binding per particle than the hard-core potential. Instead of using local soft-core potentials, one can also obtain reliable velocity-dependent potentials which also show an increase of binding in nuclear matter over hard-core potentials (KPY68). In summary, the nuclear matter calculations with local potentials seem to exclude hard-core potentials and favour soft-core potentials. The shape of the soft-core seems to be unimportant in these calculations (T67).

Calculations of H^3 and He^3

In order to choose between potentials that yield the same two-body scattering results, and similar results in nuclear matter, an accurate few-body calculation may be the decisive factor. The simplest few-body problem besides the deuteron is the three-nucleon system, H^3 or He^3. The results of Davies (D67) and Delves and Blatt (DB67) of their calculation with realistic hard-core potentials are upper bounds to the ground state energy of the triton, which are about 3MeV above the actual ground state energy. The discrepancy may be reduced somewhat by improving the trial wave function in the variational calculation and by including effects due to three-body forces and relativistic energies. On the other hand, one would also expect the replacement of the hard-core by a soft-core to have some influence on the triton, since the triton is a more tightly bound system than the deuteron and consequently it would be affected more by the short range behaviour of the nucleons.

That the suppression of the wave function at small interparticle distances is desirable in He^3 and the triton is also evident from the various studies on elastic and inelastic electron scattering from He^3 and H^3 and two-body photodisintegration and π^- capture by He^3 (G67; K67; C66).

In those calculations the wave function describes three-body states in which particles have very small probability of coming close to each other. In all cases, the suppression of the wave function is smooth, i.e. the wave function falls off to become small but finite close to zero interparticle distance. This is the kind of behaviour a soft-core potential would produce. These calculations do not exclude hard-core type wave functions but they do indicate that in the areas where the calculations are sensitive to short-range correlation, the experimental data are consistent with soft-core type correlation. It should also be noted that whereas Khanna (K67) and Cheon (C66) use proper correlation functions of Gaussian or exponential types, i.e. $1-e^{-\beta r^2}$ or $1-e^{-\beta_o r}$, with r being the distance between particles, Gibson's mechanism (G67) involves the use of a multiplicative factor, R^n, $n \geq o$ for small R where $R = \sqrt{r_1^2 + r_2^2 + r_3^2}$. Gibson's wave function is not as restrictive, and perhaps somewhat unrealistic in the sense that it vanishes when all three-interparticle distances vanish but remains finite when one distance becomes zero and the other two are non-zero.

Another property of the nuclear force that is not uniquely defined by two-body data fitting is the ratio of tensor-to-central force. In low energy systems, this would mean especially the $^3S_1$ and $^3D_1$ mixture. It is found in nuclear matter that the tensor-to-central ratio is important to obtain saturation at the correct density (SBD66; S67). It was suggested that the reason for underbinding of nuclear matter with realistic local potentials is the large tensor-to-central force ratio, and that a weaker ratio would give more binding.

For attractive potentials, it has been known for a long time that purely central forces giving the correct deuteron binding lead to excessive binding of the triton and the alpha particle (I51; BW52; p. 201). Calculations with purely attractive forces which include both central and tensor components are able to give reasonable triton binding (PF52) albeit the Coulomb radius is still too small. Ohmura *et al*. (KMY56; KMY57; O59) have shown that the inclusion of hard repulsive cores in purely central forces will give reasonable values for the binding of the triton and the Coulomb energy of He^3 when they use core radii consistent with those used in realistic phenomenological potentials. The same calculations were done more accurately by Y. C. Tang *et al*. (TSH65), van Wageningen and Kok(VK67) and Rosati and Barbi (RB66). They came to the same conclusion. A calculation by Blatt and Derrick (BD58) gives a result concerning both the repulsive core and the tensor force contribution to the triton binding. Their conclusion is that as the core radius in the potential is increased, the effectiveness of the tensor force in binding the triton decreases. There is a definite correlation between core sizes and the effect of the tensor force in binding the triton.

The three-nucleon system is the smallest and hence the least complex of nuclear systems that may involve many-body forces, as distinct from two-body forces. When a calculation of the three-body system is done with realistic forces and when the calculation as well as the potential are known to be reliable, the discrepancy between theory and experiment would indicate the relative importance of three-body forces. Normally one assumes that only two-body forces act in doing nuclear structure calculations, with the hope that if three-body and many-body forces do exist they are unimportant and can be neglected or treated as a perturbation. Nuclear forces predicted from meson theory must include short-range many-body forces. Estimates have been made of their effect in the three-nucleon system. Loiseau and Nogami (LN67) have shown that they may have an appreciable effect on the binding of the triton, i.e. of the order of 1MeV greater binding. Pask (P67) has done a perturbation calculation with the wave function obtained by Davies (D67) for the Hamada-Johnston potential, which indicates that three-body forces may increase the binding by as much as 1.5MeV; this is a large percentage of the total binding but a small percentage of the total potential energy, thus justifying the perturbation theory approach.

Throughout the calculation we assume that the triton can be treated non-relativistically. Relativistic corrections are thought to be more important in the triton than in the deuteron, mainly because the triton is more tightly bound than the deuteron. But the total internal kinetic energy of the system turns out to be less than 100MeV (DB67). For that reason, we expect high energy scattering processes between nucleons to be rare so that the potential model is valid in most instances. Gupta *et al.* (GBM65) have calculated the relativistic correction to a triton binding calculation with separable potentials. Their correction increases the binding of triton by .5MeV.

TABLE I-1

Recent Results for the Ground State of the Triton

Potential	Gammel-Brueckner	Hamada-Johnston	Yale
Energy	-6.60 MeV	-4.88 (-5.735)MeV	-4.64 MeV
Coulomb Energy (He^3)	.616 MeV	.549 (.58) MeV	.520 MeV
P_D%	8.8	7.7 (8.9)	6.8
R_{rms}	1.96 fm	2.32 (1.92) fm	2.44 fm

These results are from Delves and Blatt (DB67) except those in brackets, which give an improvement by Davies (D67).

TABLE I-2

Experimentally Determined Quantities for the Ground State of H^3 and He^3

Nucleus	H^3	He^3	
Energy	$-8.48192 \pm .00020$ MeV	$-7.71808 \pm .00017$ MeV	(MTW67)
Coulomb Energy		$.7638 \pm .0001$ MeV	(MTW67a)
P_d%	∿4%*	∿4%*	(V57)
$r_{magnetic}$	$1.70 \pm .05$ fm	$1.74 \pm .10$	(CHHJYDW65)
r_{charge}	$1.70 \pm .05$ fm	$1.87 \pm .05$	

* The D-state probability is calculated very crudely from magnetic moment considerations. Exchange effects are likely more dominant in the triton than in the deuteron because the triton has smaller size (P62, p.83; S53, chapter 9). D-state probabilities anywhere between 2% and 8% would not be inconsistent with experiment.

Intent of This Work

In this thesis we attempt to formulate the three-body problem as a variational calculation for the soft-core Reid and Bressel-Kerman potentials. We do this by choosing a simple trial function which does include the most important components of the ground state of the triton, viz. the symmetric S-state, mixed symmetry S-state, symmetric P-state, and the symmetric D-state. The goodness of the wave function is tested by applying it to the Pease-Feshbach potential (PF52) for which accurate calculations have been done (BDL62). This potential includes a tensor part but is completely attractive. To separate the effects of the soft-core of the potential, a model calculation is done with a central potential with a soft-core of Yukawa shape (CY63). For this potential calculations are done with two kinds of trial functions, a superposition of Gaussians and a superposition of exponentials, to determine the relative accuracy with which they bind the triton. It is found that the Gaussian type function gives less binding than the exponential function for the same potential. A correction is found that should be applied to calculations of the triton binding energy with soft-core potentials. Then, calculations are done with the Reid and Bressel potentials using modified Gaussians as trial functions. Within the framework of this calculation and first order correction both potentials may bind the triton but will not overbind it.

The quantities that are calculated are the binding energy, root-mean-square radius, and the probabilities of the presence of the various states in the triton. The experimentally determined quantities are given in Table I-2.

CHAPTER II

CLASSIFICATION OF THE WAVE FUNCTION OF THE BOUND THREE-NUCLEON SYSTEM

The Derrick-Blatt and Cohen-Willis Classification

In a three-nucleon system each particle is specified by its position vector, spin, and isospin. Employing established conservation laws that apply to the ground state of the system, one can classify components of the ground state wave function according to their orbital angular momentum, intrinsic spin, isospin, and partition of the internal space function.

The center-of-mass motion of the nucleus can be eliminated by a proper choice of internal coordinates. There will be six such coordinates since the remaining three independent coordinates specify the center-of-mass position. The spatial part of the wave function, therefore, will depend on these six space coordinates only. The total angular momentum of the triton is a good quantum number; it has the experimentally determined value $J=1/2$. Since each nucleon has spin of 1/2, the two possible intrinsic spin states of the triton are $S=1/2$ or $S=3/2$. Using angular momentum addition rules, one obtains the possible orbital angular momentum states. These states are $^2S_{1/2}$, $^2P_{1/2}$, $^4P_{1/2}$, $^4D_{1/2}$, where we have used the notations $^{2S+1}L_J$. One can classify the ground state of triton in terms of these four states, in a manner analogous to the two states, $^3S_1$ and $^3D_1$, found in the deuteron.

The isospin of the ground state of the triton is 1/2, since the triton and He^3 belong to an isospin doublet. The isospin quartet states of three nucleons have higher energy than the ground state of the triton as the triproton and the trineutron are thought to be unbound systems (OD67; B67). When we consider the three-nucleon system, we will not distinguish between H^3 and He^3 but rather assume them to be two degenerate states of the same system. This assumption corresponds to the charge independence of nuclear forces. The differences between the two nuclei can be ascribed to Coulomb effects between nucleons and the mass difference of the proton and neutron. Since we also assume that nuclear forces conserve parity, we take the parity to be even. The total wave function must be antisymmetric under interchange of any pair of particles because of the Pauli exclusion principle. By combining spin, isospin, internal, and angular functions each of definite symmetry using methods prescribed by algebra or group theory, one obtains the desired antisymmetry of the wave function.

One can choose the six coordinates describing the spatial part of the wave function in various ways. Derrick and Blatt (DB58) have given a full classification of the angular momentum-isospin functions which are found in the ground state wave function of the triton. Their method involved the use of internal functions dependent on the three interparticle distances, functions dependent on the Euler angles to specify the orientation of the triangle formed by the three interparticle distances, spin functions, and isospin functions. In short, they combine spin and isospin functions to obtain spin-isospin functions. These are combined with the Euler angle functions to give total angular momentum-isospin functions, which in turn are combined with the internal functions to give an overall antisymmetric wave function.

A different approach to the complete classification of the triton states has been employed by Cohen and Willis (CW62). This classification has the advantage that it avoids Euler angles and consequently the complicated calculations that are necessary to calculate the kinetic energy. Derrick (D60) found that, with the Derrick and Blatt choice of internal coordinates, the body coordinate system is not defined when the three particles lie on a straight line or when they lie at the vertices of an equilateral triangle. He did derive a set of asymptotic conditions for these configurations to avoid diverging kinetic energy integrals.

Since the Cohen and Willis classification avoids these complications in the calculation of the kinetic energy, we will follow their approach. It turns out that with their classification we can do a variational calculation with a rather simple trial function which makes it relatively easy to calculate the kinetic energy matrix elements. This trial function also enables us to do the calculation with the Reid potential (R68) without the use of involved projection operators to project out of the total wave function those parts which have a specific two-body angular momentum dependence. With our choice of trial function, we are able to do this by inspection. A noteworthy difference between the two classifications is that in the Derrick and Blatt classification interparticle distances appear only in the internal functions, whereas in the Cohen and Willis classification they are present in the angular as well as the internal functions.

The operator method used by Cohen and Willis (CW62) is really a systematization of the approach used by Gerjuoy and Schwinger (GS42) and extended by Sachs (S53, Chapter VIII) to include isospin. In the remainder of this chapter we will describe this approach. First we will state some general results of the permutation group of three objects and then apply these results to form angular momentum-isospin functions of the system.

Permutation Symmetry

The overall wave function must be antisymmetric under the interchange of any pair of particles. In order that we may be able to keep track of the symmetry of the components of the wave function, we resort to the results of the symmetry group of degree 3, S_3 (H64, Chapter VII). There are six elements in this group (1), (123), (132), (12), (13), (23). We know that the number of nonequivalent irreducible representations of a group is equal to the number of classes in the group. The number of classes of the symmetry group of degree n can be determined by the number of partitions of n. These partitions are characterized by a set of numbers $\lambda_1, \lambda_2, \ldots$ such that

$$\lambda_1 \geqslant \lambda_2 \geqslant \lambda_3 \geqslant \cdots$$

$$\lambda_1 + \lambda_2 + \lambda_3 + \cdots = n$$

A partition is denoted by $[\lambda_1, \lambda_2, \ldots]$ and in a general way by $[\lambda]$. Thus for n=3 we have three partitions, [3], [21], and [111]. There are therefore three irreducible representations, the symmetric representation corresponding to [3], the antisymmetric representation corresponding to [111], and the mixed symmetry representation corresponding to [21]. The dimension of both the symmetric and antisymmetric representation is 1; the dimension of the mixed symmetry representation is 2. We will denote an irreducible representation by its partition $[\lambda]$. The base function of [3] is symmetric under interchange of any two objects;

similarly the base function of [111] is antisymmetric under interchange of any pair of objects. The remaining representation is spanned by two base functions one of which we take to be symmetric under the interchange of objects 1 and 2, and the other antisymmetric under the interchange of objects 1 and 2. Let us denote the function spanning the symmetric representation by ([3]), the function spanning the antisymmetric representation by ([111]), and the pair of functions spanning the mixed symmetry representation by ([21], a) and ([21], s) depending on whether the function is antisymmetric or symmetric under interchange of objects 1 and 2.

Derrick and Blatt (D58, Appendix I) have given a set of addition coefficients for combining representation base functions, analogous to Clebsch-Gordon coefficients for combining angular momentum functions. Thus, if the base functions of the representations corresponding to $[\lambda_1]$ and $[\lambda_2]$ are combined to give the K^{th} component of the base functions spanning $[\lambda]$, then

$$([\lambda], K) = \sum_{K_1, K_2} \begin{pmatrix} [\lambda_1] & [\lambda_2] & [\lambda] \\ K_1 & K_2 & K \end{pmatrix} ([\lambda_1], K_1)_1 ([\lambda_2], K_2)_2$$

The direct product of two representations of different operators acting on the same particles are decomposed into the direct sum of irreducible representations. Using the Derrick and Blatt table for the coefficients

$\begin{pmatrix} [\lambda_1] & [\lambda_2] & [\lambda] \\ K_1 & K_2 & K \end{pmatrix}$ we obtain the following results:

$$[21]_1 \otimes [21]_2 = [3] + [21] + [111]$$

$$([3]) = \frac{1}{\sqrt{2}} \{([21], s)_1 \; ([21], s)_2 + ([21], a)_1 \; ([21], a)_2\}$$

$$([21], s) = \frac{1}{\sqrt{2}} \{([21], a)_1 \; ([21[, a)_2 - ([21], s)_1 \; ([21], s)_2\}$$

$$([21], a) = \frac{1}{\sqrt{2}} \{([21], s)_1 \; ([21], a)_2 + ([21], a)_1 \; ([21], s)_2\}$$

$$([111]) = \frac{1}{\sqrt{2}} \{ -([21], s)_1 \; ([21], a)_2 + ([21],a)_1 \; ([21], s)_2\}$$

$$[21]_1 \otimes [111]_2 = [21]$$

$$([21],a) = ([21], s)_1 \; ([111])_2$$

$$([21],s) = - ([21],a)_1 \; ([111])_2$$

$$[21]_1 \otimes [3]_2 = [21]$$

$$([21], a) = ([21], a)_1 \; ([3])_2$$

$$([21], s) = ([21], s)_1 \; ([3])_2$$

$[3]_1 \otimes [111]_2 = [111]$ $\qquad$ $([111]) = ([3])_1 \; ([111])_2$

$[3]_1 \otimes [3]_2 = [3]$ $\qquad$ $([3]) = ([3])_1 \; ([3])_2$

$[111]_1 \otimes [111]_2 = [3]$ $\qquad$ $([3]) = ([111])_1 \; ([111])_2$

The one-dimensional product representations are obvious but for completeness we have included them. The above results can also be obtained if one uses algebraic methods on functions which are initially defined to possess one of the three symmetries. One observes what effect the different exchange operators have on the functions and also what effect they have on certain linear combinations of products of these functions. This is the approach used by Sachs (S53, Chapter VIII), by Schiff (S64), and by Gibson and Schiff (GS65).

We saw earlier that the ground state of the triton consists of a combination of LSJ states. Each of the four LSJ states can be subdivided into states which are base functions of irreducible representations of S_3. The components of the ground state of the triton are therefore labelled by ${}^{2S+1}L_J$ and the partition of S_3 of which the component is a base function.

Operational Representation

Using the "operational representation" procedure we can systematically derive all the possible orbital angular momentum and symmetry states. First, we define a spin function with S=1/2 and an isospin function with T=1/2. Since the triton is a state with J=1/2 and T=1/2 we operate on the product of the spin and isospin function with scalar functions of the spin vector operators and the space vectors of the system. We can do this without changing the total angular momentum of the nucleus because such functions commute with J^2. In forming the scalar functions we must keep track of the symmetry. Such rotationally invariant functions can only be formed by combining the scalars, vectors, and tensors made up from spin operators with similar forms made up from the position vectors. Similarly, on our basic function we can operate with a scalar function of the isospin operators because it commutes with T^2.

(i) Spin and Isospin Functions

The total intrinsic spin of the system is either 1/2 or 3/2. As our basic spin state we take the function, with S=1/2,

$$\phi = \frac{1}{\sqrt{2}} (\alpha_1\beta_2 - \alpha_2\beta_1)\alpha_3.$$

In this spin state particles 1 and 2 have total spin 0, and the spin of ϕ is determined completely by the third particle. ϕ is one component of the functions spanning the mixed representation of S_3. Both functions are

$$\phi \equiv \phi^{(1/2)}([21], a) = \frac{1}{\sqrt{2}} (\alpha_1\beta_2 - \alpha_2\beta_1)\alpha_3$$

$$\phi^{(1/2)}([21], s) = \sqrt{\frac{2}{3}} [1/2(\alpha_1\beta_2+\alpha_2\beta_1)\alpha_3-\alpha_1\alpha_2\beta_3]$$

where we have indicated the symmetry properties. The latter function can also be written in terms of the spin operators $\vec{\sigma}^{(1)}$ and $\vec{\sigma}^{(3)}$ acting on ϕ, i.e.

$$\phi^{(1/2)}([21], s) = -\frac{1}{\sqrt{3}} (\vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(3)})\phi$$

The operators $\vec{\sigma}^{(1)}$ and $\vec{\sigma}^{(2)}$ operating on ϕ are not linearly independent; in fact, because of the antisymmetry of the spins of particles 1 and 2, $\vec{\sigma}^{(1)}\phi = -\vec{\sigma}^{(2)}\phi$. Therefore, we need to use only $\vec{\sigma}^{(1)}$ and $\vec{\sigma}^{(3)}$ as spin operators acting on ϕ. We have now exhausted the scalar spin operators that can be found to act on ϕ so that linearly independent states are produced. The above two spin functions can be used with the orbital angular S-state and, of course, will then give total $J=1/2$ and $M_J=1/2$.

There are three independent spin vector operators, namely $\vec{\sigma}^{(1)}$, $\vec{\sigma}^{(3)}$, and $\vec{\sigma}^{(1)} \times \vec{\sigma}^{(3)}$ (independent in the sense that independent spin functions are formed when they act on ϕ) which may be combined with orbital angular P-states to give scalars operating on ϕ. However, we want to form these three spin vector operators acting on ϕ so that the resulting forms are base functions of representations of the symmetry group. If we operate with $(\vec{\sigma}^{(1)} + \vec{\sigma}^{(2)} + \vec{\sigma}^{(3)})$ on the S-state spin functions, we obtain two vector spin functions, each of which we write in terms of an arbitrary Cartesian component

$$\phi_i^{(1/2)}([21], a) = i\,\sigma_i^{(3)}\phi$$

$$\phi_i^{(1/2)}([21], s) = -\frac{1}{\sqrt{3}}\{i\sigma_i^{(1)} + (\vec{\sigma}^{(1)} \times \vec{\sigma}^{(3)})_i\}\phi$$

These functions are defined except for an arbitrary phase factor. They have spin 1/2, as did the S-state functions, since $(\vec{\sigma}^{(1)} + \vec{\sigma}^{(2)} + \vec{\sigma}^{(3)})$ commutes with $(\vec{\sigma}^{(1)} + \vec{\sigma}^{(2)} + \vec{\sigma}^{(3)})^2$, and the symmetry is unaltered since the operator is symmetric under interchange of spins. To obtain the third spin vector we make the observation that the two spin vectors already obtained span the mixed symmetry representation; the third vector must span a one-dimensional representation, either the symmetric or the antisymmetric. It is impossible to combine the three spins, each of which has only two states, into an antisymmetric configuration. Thus, the last vector must be symmetric. Let us apply the spin operators spanning a mixed symmetry representation to the S-state functions so as to give a symmetric spin function. Such spin operators are

$$\vec{S}([21], a) = \frac{1}{\sqrt{2}} [\vec{\sigma}^{(2)} - \vec{\sigma}^{(1)}]$$

$$\vec{S}([21], s) = \sqrt{\frac{2}{3}} [\vec{\sigma}^{(3)} - 1/2(\vec{\sigma}^{(1)} + \vec{\sigma}^{(2)})]$$

Performing this operation and normalizing the resulting function gives us

$$\phi_i^{(3/2)}([3]) = \sqrt{\frac{2}{3}} \{i\sigma_i^{(1)} - 1/2(\vec{\sigma}^{(1)} \times \vec{\sigma}^{(3)})_i\}\phi$$

The three P-state spin functions are orthonormal. One can show that the last function represents a quartet state by acting on it with the operator $(\vec{\sigma}^{(1)} + \vec{\sigma}^{(2)} + \vec{\sigma}^{(3)})^2$.

The spin state that combines with the orbital angular momentum D-state must be a quartet state. Therefore, it must be symmetric and transform like a spherical harmonic of second order. A traceless symmetric second rank tensor formed from two vectors is such a quantity since it has that transformation property. We form the spin D-state by combining the Cartesian vector components of the symmetric operator $(\vec{\sigma}^{(1)} + \vec{\sigma}^{(2)} + \vec{\sigma}^{(3)})_i$ with the vector components of $\phi_j^{(3/2)}([3])$ to give a traceless symmetric second rank tensor which after simplification and normalization becomes

$$\phi_{ij}^{(3/2)}([3]) = 1/2(\sigma_i^{(1)}\sigma_j^{(3)} + \sigma_j^{(1)}\sigma_i^{(3)} - 2/3\ \delta_{ij}\ \sigma_k^{(1)}\sigma_k^{(3)})\phi$$

As before, since the operator commutes with $(\vec{\sigma}^{(1)} + \vec{\sigma}^{(2)} + \vec{\sigma}^{(3)})^2$, the spin is unchanged. This state could also have been obtained in a different way, e.g. by combining components of the vector operators $\vec{S}([21], a)$ and $\vec{S}([21], s)$ with the doublet spin P-function in such a way as to obtain a symmetric function. Then, however, one would have to check the total spin of such a function. The manner in which the spin function is found is not unique, but the number of independent spin functions is, and that is determined by the number of linearly independent spin operators at our disposal.

The isospin state of the triton is T=1/2, T_3= -1/2. Analogous to the intrinsic spin S=1/2 state of the triton, we find that there are two isospin functions spanning a mixed symmetry representation

$$\chi([21], a) = \frac{1}{\sqrt{2}} (\xi_1{}^{+} \xi_2{}^{-} - \xi_1{}^{-} \xi_2{}^{+})\xi_3{}^{-}$$

$$\chi([21], s) = -\frac{1}{\sqrt{3}} (\vec{\tau}^{(1)} \cdot \vec{\tau}^{(3)})\chi([21], a)$$

Since we assume the triton and He^3 to be states of isospin T=1/2, these are the only functions we need. For the He^3 isospin function, the third nucleon has a third component of isospin $\xi_3{}^{+}$. If we wish to include in the problem effects which are due to the charge dependence of nuclear forces and calculate their magnitude, or if we want to build up scattering states, we would be forced to include T=3/2 functions, and our analysis for isospin would be more involved. Since we assume a charge independent and space symmetrical system, our analysis is the same whether $T_3 = +1/2$ or $-1/2$ or whether $M_J = +1/2$ or $-1/2$. The energy difference between He^3 and H^3 can be calculated in two different ways. One can include T=3/2 components in the He^3 wave function and do a calculation with the nuclear plus Coulomb force. On the other hand, since the Coulomb force is weak compared to the nuclear force, we can use the pure T=1/2 wave function found in a triton calculation as an unperturbed wave function to find the energy shift by means of first order perturbation theory.

(ii) Space Functions

To specify the spatial configuration of the system after the removal of the center-of-mass coordinates, we define the two vectors

$$\vec{\rho} = \frac{1}{\sqrt{2}} (\vec{r}_2 - \vec{r}_1) \qquad ([21], a)$$

$$\vec{r} = \sqrt{\frac{2}{3}} [\vec{r}_3 - 1/2(\vec{r}_1 + \vec{r}_2)] \qquad ([21], s)$$

where $\vec{r}_1$, $\vec{r}_2$, and $\vec{r}_3$ are the position vectors of the nucleons. The two vectors, $\vec{\rho}$ and $\vec{r}$, span a mixed representation of the symmetry group. In order to build up possible orbital angular momentum states we have to bear in mind that the triton and He^3 are even parity systems. Vectors change sign under the inversion of the coordinate system, scalars, which include scalar products of vectors, do not. The cross product of two vectors is a pseudovector which has even parity. In general, traceless symmetric tensors formed from Cartesian components of vectors have even parity if the rank of the tensor is even, and odd parity if the rank is odd. The tensors constructed from axial vectors always have even parity. When the tensor is constructed from r vectors and an arbitrary number of axial vectors, the parity of the tensor is $(-1)^r$.

In order to form S-states of different symmetry, we see that we can combine the vectors into three linearly independent scalars:

$$\rho^2 + r^2 \qquad ([3])$$

$$2\vec{\rho}\cdot\vec{r} \qquad ([21], a)$$

$$\rho^2 - r^2 \qquad ([21], s)$$

With our choice of vectors it is difficult to see that an antisymmetric S-state exists. But if one considers the three scalar functions u, v, and w of a vector, it is obvious that the function

$$f(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \begin{vmatrix} u(\vec{r}_1) & v(\vec{r}_1) & w(\vec{r}_1) \\ u(\vec{r}_2) & v(\vec{r}_2) & w(\vec{r}_2) \\ u(\vec{r}_3) & v(\vec{r}_3) & w(\vec{r}_3) \end{vmatrix}$$

is antisymmetric under the interchange of any two particles.

For the P-state the only even parity vector that can be found is $(\vec{\rho} \times \vec{r})_i = \varepsilon_{ijk}\rho_j r_k$. This vector is antisymmetric, i.e. it belongs to [111]. In order to form D-states we see that as with the S-state scalars, we can form three traceless symmetric tensors of second rank which are linearly independent:

$$T_{ij}([3]) = T_{ij}(\rho, \rho) + T_{ij}(r, r) \qquad ([3])$$

$$T_{ij}([21], a) = 2\, T_{ij}(\rho, r) \qquad ([21], a)$$

$$T_{ij}([21], s) = T_{ij}(\rho, \rho) - T_{ij}(r, r) \qquad ([21], s)$$

where $T_{ij}(a, b) = 1/2\ [a_i b_j + a_j b_i - 2/3\ \delta_{ij}(\vec{a}\cdot\vec{b})]$. We can multiply the P and D functions by any S-state function without changing the angular momentum, e.g. we can form an antisymmetric D-state, $f(\vec{r}_1, \vec{r}_2, \vec{r}_3)\ T_{ij}\ ([3])$.

(iii) Overall Wave Function

We are now in a position to write down the angular momentum states classified according to the partition of the function. These functions must be combined with a scalar function of the symmetry necessary to form an overall antisymmetric function. Such scalar functions are denoted as internal functions and we will mention their symmetry when referring to a state belonging to a particular classification, e.g. the symmetric D-state is one which has orbital angular momentum equal to two and whose angular-isospin function is antisymmetric. In forming the angular-isospin function we must use the rules of combining base functions of representations of the symmetry group S_3, and we must ensure that the operator acting on ϕ and χ is a scalar. We list the angular-isospin function as found in Cohen and Willis' paper (CW62) except for changes in phase.

TABLE II-1

<u>S-state</u> <u>Symmetry</u>

$$\begin{aligned} Y_1 = \frac{1}{\sqrt{2}} [&\phi^{(1/2)}([21], a)\chi([21], s) \\ &- \phi^{(1/2)}([21), s)\chi([21], a)] \qquad ([111]) \end{aligned}$$

$$\begin{aligned} Y_2 = \frac{1}{\sqrt{2}} [&\phi^{(1/2)}([21], a)\chi([21], a) \\ &+ \phi^{(1/2)}([21], s)\chi([21], s)] \qquad ([3]) \end{aligned}$$

$$\begin{aligned} Y_{3,a} = \frac{1}{\sqrt{2}} [&\phi^{(1/2)}([21], a)\chi([21], s) \\ &+ \phi^{(1/2)}([21], s)\chi([21], a)] \qquad ([21], a) \end{aligned}$$

$$\begin{aligned} Y_{3,s} = \frac{1}{\sqrt{2}} [&\phi^{(1/2)}([21], a)\chi([21], a) \\ &- \phi^{(1/2)}([21], s)\chi([21], s)] \qquad ([21], s) \end{aligned}$$

P-state — Symmetry

$$Y_4 = \frac{1}{\sqrt{2}} [\phi_i^{(1/2)}([21], a)\chi([21], a) + \phi_i^{(1/2)}([21], s)\chi([21], s)](\vec{\rho} \times \vec{r})_i \qquad ([111])$$

$$Y_5 = \frac{1}{\sqrt{2}} [\phi_i^{(1/2)}([21], a)\chi([21], s) - \phi_i^{(1/2)}([21], s)\chi([21], a)](\vec{\rho} \times \vec{r})_i \qquad ([3])$$

$$Y_{6,a} = \frac{1}{\sqrt{2}} [\phi_i^{(1/2)}([21], a)\chi([21], a) - \phi_i^{(1/2)}([21], s)\chi([21], s)](\vec{\rho} \times \vec{r})_i \qquad ([21], a)$$

$$Y_{6,s} = \frac{1}{\sqrt{2}} [\phi_i^{(1/2)}([21], a)\chi([21], s) + \phi_i^{(1/2)}([21], s)\chi([21], a)](\vec{\rho} \times \vec{r})_i \qquad ([21], s)$$

$$Y_{7,a} = \phi_i^{(3/2)}([3])\chi([21], s)(\vec{\rho} \times \vec{r})_i \qquad ([21], a)$$

$$Y_{7,s} = -\phi_i^{(3/2)}([3])\chi([21], a)(\vec{\rho} \times \vec{r})_i \qquad ([21], s)$$

D-state

$$Y_8 = \frac{1}{\sqrt{2}} \phi_{ij}^{(3/2)}([3]) [\chi([21], a)T_{ij}([21], s) - \chi([21], s)T_{ij}([21], a)] \qquad ([111])$$

$$Y_9 = \frac{1}{\sqrt{2}} \phi_{ij}^{(3/2)}([3]) [\chi([21], a)T_{ij}([21], a) + \chi([21], s)T_{ij}([21], s)] \qquad ([3])$$

$$Y_{10,a} = \phi_{ij}^{(3/2)}([3])\chi([21], a)T_{ij}([3]) \qquad ([21], a)$$

$$Y_{10,s} = \phi_{ij}^{(3/2)}([3])\chi([21], s)T_{ij}([3]) \qquad ([21], s)$$

D-state (cont'd) Symmetry

$$Y_{11,a} = \frac{1}{\sqrt{2}} \phi_{ij}^{(3/2)}([3])\ [\chi([21],\ a)T_{ij}([21],\ s) + \chi([21],\ s)T_{ij}([21],\ a)] \qquad ([21],\ a)$$

$$Y_{11,s} = \frac{1}{\sqrt{2}} \phi_{ij}^{(3/2)}([3])\ [\chi([21],\ a)T_{ij}([21],\ a) - \chi([21],\ s)T_{ij}([21],\ s)] \qquad ([21],\ s)$$

Summation over repeated subscripts is implied.

The ground state wave function is written

$$\Psi = Y_i f_i$$

If we take the Y_i's in the order they appear in Table II-1, then the f_i's are to be taken in the following order: f_1, f_2, $f_{3,s}$, $-f_{3,a}$, f_4, f_5, $f_{6,s}$, $-f_{6,a}$, $f_{7,s}$, $-f_{7,a}$, f_8, f_9, $f_{10,s}$, $-f_{10,a}$, $f_{11,s}$, $-f_{11,a}$. The two component f_i's are of mixed symmetry as indicated, f_1, f_4, and f_8 are symmetric functions, and f_2, f_5, and f_9 are antisymmetric functions. Derrick and Blatt (DB58) originally obtained only ten angular-isospin functions, i.e. three mixed symmetry D-states instead of four D-states, two of which are of mixed symmetry, one antisymmetric and the remaining one symmetric. However, Derrick (D60a) has shown that the three D-states of Derrick and Blatt are equivalent to four D-states of the symmetry types of Cohen and Willis. This indicates the equivalence of the two classifications.

CHAPTER III

CALCULATIONS OF MATRIX ELEMENTS WITH REALISTIC FORCES

Exact Solution of the Three-Nucleon Problem

To solve the three-body Schrödinger equation with "realistic" local potentials which contain central, tensor, L•S, and quadratic (L•S) terms, is a problem of such numerical magnitude that as yet this has not been attempted. Since the spatial part of the three-body Hamiltonian depends on six-coordinates, one must solve a second order partial differential equation in six independent variables. A simplification much like that used to reduce the deuteron problem to manageable form, is possible to minimize the complexity of the exact solution of the triton.

In the deuteron case one must solve the two-particle Schrödinger equation which consists of a partial differential equation in three independent variables. But the deuteron wave function can be expressed as the sum of $^3S_1$ and $^3D_1$ components. It is the orthogonality of these two angular functions that results in the reduction of the problem to two coupled differential equations in one variable, which are easily solvable. The coupling of the two equations, or states, is due to the presence of the tensor force. If there is no tensor force, one has to solve one differential equation in one unknown.

In both the Derrick and Blatt classification and the Cohen and Willis classification of the triton states, there are sixteen orthogonal angular momentum-isospin functions. The angular functions are determined by three of the six coordinates necessary to determine the spatial part of the wave function. Thus, if one operates with the three-body Hamiltonian on the total wave function and takes the scalar product with each of the sixteen angular momentum-isospin functions separately, he will obtain sixteen coupled second order differential equations in three independent variables. The reason for this being so is that the matrix elements of the kinetic energy operator and the potential energy operators between angular momentum-isospin functions can be evaluated exactly (D60; CW62). The tensor force is still the mechanism by which states of different orbital angular momentum are coupled. In the absence of the tensor force, the number of differential equations becomes four and the ground state of the triton is a pure ${}^2S_{1/2}$ state. If the forces are not only central, but also spin-independent, then the problem reduces to one differential equation in three unknowns. Of the three ${}^2S_{1/2}$ states Derrick and Blatt (DB58) have pointed out, the symmetric S-state would be the dominant component of the ground state since the antisymmetric S-state and the mixed symmetry S-state would have more kinetic energy associated with them. Even in the case of the simplest force, which is known to be quite unrealistic, the solution of a second order differential equation in three unknowns must be found. To date, even this equation is solved only by making approximations.

Equivalent Two-Body Methods

Since the two-body bound state problem is completely solvable in the non-relativistic limit, it seems natural to try to formulate the triton problem in such a way that the solution depends on equations which are similar to the deuteron equation. This is first done with the simplest triton model, viz. triton whose ground state is a symmetric S-state, with the hope that the method can be extended to all triton states. Rather than using a spin-independent potential for this case, it is possible in the first approximation to use a force acting between the nucleons which is the arithmetic average of spin-singlet and spin-triplet forces (BW52, pp. 194-5) acting only in even orbital angular momentum states. We denote these forces as singlet-even and triplet-even respectively. The argument is as follows. The nucleons can only interact via even orbital angular momentum states in order to preserve the total symmetry of the system. The two neutrons are in a spin-singlet state, one neutron-proton pair is in a spin triplet state and the other neutron-proton pair is a mixture of equal amounts of singlet and triplet states. The average force per bond is then $1/2\ (V_{t,e} + V_{s,e})$.

The usual method of solving the problem of triton or He^3 in the symmetric S-state is some kind of equivalent two-body method. Basically this amounts to reducing the problem of three particles to a differential equation which is very similar to the two-body Schrödinger equation. Wigner (W33) initiated this approach by assuming that the force between the neutrons is zero, and that the wave function is separable in the remaining two coordinates. Feshbach and Rubinow (FR55) and Morpurgo (M52) have formulated equivalent two-body methods by restricting the three spatial degrees of freedom to a single one in the action integral and then writing down the Euler-Lagrange equation of the action. This gives a second order differential equation in one independent variable. Feshbach and Rubinow used as their one coordinate $R = 1/2(r_{12} + r_{23} + r_{31})$ after Feshbach (BW52, p. 196) found that $e^{-1/2\ K(r_{12} + r_{23} + r_{31})}$ is an excellent trial wave function in a variational calculation for this simple triton model. Morpurgo uses as independent variable $R = \sqrt{1/3(r_{12}^2+r_{23}^2+r_{31}^2)}$ and also obtained a Schrödinger type differential equation. According to McMillan (M65) the same differential equation is obtained if one lets $R^2 = r_{12}^2 + r_{23}^2 + r_{31}^2$. McMillan has shown the superiority of the Feshbach-Rubinow equation over the Morpurgo equation by virtue of the fact that both equations are derived from a variational principle and hence must yield an upper bound to the eigenenergy. For identical potentials of the exponential or Yukawa type the Morpurgo equation yields a higher upper bound than the Feshbach-Rubinow equation. Recently, McMillan and Best (MB67) have extended the Feshbach-Rubinow method to include the symmetric D-state. They were able to do a calculation with the tensor term in the potential. Although their work is encouraging, it is a long way yet from the inclusion of all states found in triton. Furthermore, for potentials with a hard or soft core causing short range correlations between nucleons, the method breaks down since the coordinate $R = 1/2(r_{12} + r_{23} + r_{31})$ does not distinguish between configurations where r_{12} is small and r_{23} and r_{31}, fairly large, or all three distances approximately equal. With short range repulsion, the wave function should be zero or near zero in the former instance, and should have finite amplitude in the latter. If one wants to extend this method to mixed symmetry states and/or antisymmetric states, then the single coordinate will have to be replaced by several coordinates of the type $R = 1/2\ (\eta_3\ r_{12} + \eta_1\ r_{23} + \eta_2\ r_{13})$ where η_i's are not all equal but do have definite values. When the η_i's are not equal it has been shown that as the asymmetry factors become larger the method gives poorer results (BNV67). It does not appear, therefore, that an extension of this method will lead to a satisfactorily complete calculation of the triton.

Further developments along the lines of two-body methods for three-body problems have been made. Delves and Derrick (DD63) use the angular-isospin functions of Derrick and Blatt (DB58) and internal functions of the form $u(r_{12})v(r_{23})w(r_{31})$ in order to obtain a set of coupled differential equations for the two most important S-states and the three D-states. They obtain eight coupled differential equations in one variable. Unfortunately these equations also have a set of variational parameters which must be determined before an upper bound to the solution is obtained.

Bodmer and Shamsher Ali (BA64) have developed a similar method for only the S-state without taking into account the triton antisymmetry, although the calculation is the same for the symmetric S-state. They consider ${}_{\Lambda}Be^{9}$ as a three-body problem consisting of two alpha particles and one lambda particle. Their spatial wave function is of the form $g_1(r_{12})g_2(r_{23})g_3(r_{31})$ and inserting this form in the action integral, they find a set of three coupled integro-differential Euler-Lagrange equations by varying with respect to the g_i's. Rosati and Barbi (RB66) have shown that with present day computers one can very efficiently obtain numerical solutions to these equations. By making the g_i's of the same form, one has probably the most accurate practical method of solving for the triton symmetric S-state. Murphy and Rosati (MR65) have shown that Bodmer and Ali's method can be extended to arbitrary angular momentum states. However, they do not take account of the exclusion principle in their wave function; it would be very tedious to project out states that are completely antisymmetric under exchange of coordinates.

Variational Calculation

(i) Trial Wave Function

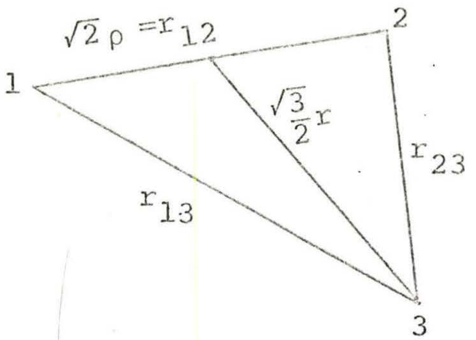
The equivalent two-body methods are unsuitable for calculations with a realistic local force because the resultant equations either have lost the essential features in the simplification of the problem or else they are still practically unsolvable. To date, therefore, the only accurate calculations with realistic potentials have been done using the Rayleigh-Ritz variational method. This is the approach that we will follow. Our first task is to choose a trial function which has the correct symmetry, and angular momentum. There are, of course, other conditions that it must satisfy. The trial function must be localized, i.e. as two of the particles move far apart it must tend to zero as then the triton bound state no longer exists. If the two-particle force is infinite at the origin the wave function must tend to zero when the particles come very close together. As shown in the previous chapter, we have a set of functions with the angular momentum and symmetry character for the different states found in the triton. Such a function can always be multiplied by a totally symmetric function without changing the symmetry of the original function, and if at the same time the multiplying function is a scalar then the angular momentum character of the function is unchanged. If we restrict the function even more so that it is a scalar in the two-body system, then the angular momentum in that particular two-body system is unchanged.

The three particles are fixed in space by the vectors $\vec{r}_1$, $\vec{r}_2$, and $\vec{r}_3$. The system in the center-of-mass frame can be specified by the vectors

$$\vec{\rho} = \frac{1}{\sqrt{2}} (\vec{r}_2 - \vec{r}_1)$$

$$\vec{r} = \sqrt{\frac{2}{3}} \{\vec{r}_3 - 1/2(\vec{r}_1 + \vec{r}_2)\}.$$

$(\rho^2 + r^2)$ is a scalar quantity that is totally symmetric under interchange of any pair of particles. Thus, the Gaussian function $e^{-\lambda(\rho^2 + r^2)}$ seems to satisfy the symmetry requirement. It is also a three-body scalar as well as a scalar in the system of particles one and two since they are related only through ρ^2. No angular coordinates are present. If, on the other hand, we consider the exponential function $e^{-\lambda(r_{12} + r_{13} + r_{23})}$ which is used quite often in variational calculations, we find that it satisfies all our requirements except that it be a scalar in the two-body coordinate system. Consider r_{12} (from symmetry we could pick any one of the three variables)



$$r_{12} = \sqrt{2}\,\rho$$

$$r_{13} = \sqrt{\frac{1}{2}\rho^2 + \frac{3}{2}r^2 + \sqrt{3}\,(\vec{\rho}\cdot\vec{r})}$$

$$r_{23} = \sqrt{\frac{1}{2}\rho^2 + \frac{3}{2}r^2 - \sqrt{3}\,(\vec{\rho}\cdot\vec{r})}$$

Thus $e^{-\lambda(r_{12} + r_{13} + r_{23})} = e^{-\lambda f[\rho^2,\, r^2,\, (\vec{\rho}\cdot\vec{r})]}$. The exponential now is not only dependent on ρ^2 and r^2 but also on $(\vec{\rho}\cdot\vec{r})$, i.e. the angle between $\vec{\rho}$ and $\vec{r}$. It is this angular dependence that introduces angular momentum components other than L = 0. This makes the exponential function unsuitable for analytically separating out the two-body angular momentum components. This is a necessity for calculations with the Reid potential.

For our calculation we have only used those states which we feel will be the most important three-body states, namely the symmetric S-state (S), the mixed symmetry S-state (S'), the symmetric P state (P), and symmetric D-state (D). The wave function was chosen mainly to include states having the least amount of kinetic energy and at the same time enabling the function to use the tensor part of the potential to the fullest extent. A function with no or few nodes has less kinetic energy associated with it than a function with several nodes. Derrick and Blatt (DB58) have given a qualitative argument for estimating the importance of the kinetic energy contribution. If we consider the triangle formed by the three inter-particle distances, then the wave function does not have to vanish for any shape of the triangle when the function is totally symmetric; when there is a pair of functions of the mixed symmetry type, the functions are zero when the triangle is equilateral, and an antisymmetric function is necessarily zero when the triangle is isosceles. We have included the P-state because it is easy to include but we expect its presence to have very little influence on the total binding. The omitted states can be included by a perturbation treatment applied to the variational function.

The spatial parts of the trial wave functions used are given below. We also give the representation of the group S_3 that they span as well as the three-body orbital angular momentum.

$$\psi_1 = \sum_i a_i^{(1)} \frac{(2\lambda_i^{(1)})^{3/2}}{\pi^{3/2}} e^{-\lambda_i^{(1)}(\rho^2+r^2)} \qquad [3] \quad S$$

$$\psi_{2a} = 2(\vec{\rho}\cdot\vec{r}) \sum_i a_i^{(2)} \frac{(2\lambda_i^{(2)})^{5/2}}{\pi^{3/2}} e^{-\lambda_i^{(2)}(\rho^2+r^2)}$$

$$[21] \quad S'$$

$$\psi_{2s} = (\rho^2-r^2) \sum_i a_i^{(2)} \frac{(2\lambda_i^{(2)})^{5/2}}{\pi^{3/2}} e^{-\lambda_i^{(2)}(\rho^2+r^2)}$$

$$\psi_3^j = (\vec{\rho} \times \vec{r})_j \sum_i a_i^{(3)} \frac{(2\lambda_i^{(3)})^{5/2}}{\pi^{3/2}}$$

$$\times\, e^{-\lambda_i^{(3)}(\rho^2+r^2)} \qquad [111] \quad P$$

$$\psi_{4a}{}^{jk} = 2\ T_{jk}(\rho,r)\ \sum_i a_i^{(4)}\ \frac{(2\lambda_i^{(4)})^{5/2}}{\pi^{3/2}} \times e^{-\lambda_i^{(4)}(\rho^2+r^2)}$$

[21] D

$$\psi_{4s}{}^{jk} = [T_{jk}(\rho,\rho) - T_{jk}(r,r)] \sum_i a_i^{(4)}\ \frac{(2\lambda_i^{(4)})^{5/2}}{\pi^{3/2}} \times e^{-\lambda_i^{(4)}(\rho^2+r^2)}$$

$$\psi_5 = (\vec{\rho} \times \vec{r})^2 \sum_i a_i^{(5)}\ \frac{(2\lambda_i^{(5)})^{7/2}}{\pi^{3/2}} \times e^{-\lambda_i^{(5)}(\rho^2+r^2)}$$

[3] S

$$\psi_6 = (\vec{\rho} \times \vec{r})^4 \sum_i a_i^{(6)}\ \frac{\sqrt{70}}{5 \times 7 \times 9}\ \frac{(2\lambda_i^{(6)})^{11/2}}{\pi^{3/2}} \times e^{-\lambda_i^{(6)}(\rho^2+r^2)}$$

[3] S

$$\psi_{7a}{}^{jk} = (\vec{\rho} \times \vec{r})^2\ 2T_{jk}(\rho,r) \sum_i a_i^{(7)}\ \frac{1}{\sqrt{385}} \times \frac{(2\lambda_i^{(7)})^{9/2}}{\pi^{3/2}}\ e^{-\lambda_i^{(7)}(\rho^2+r^2)}$$

[21] D

$$\psi_{7s}{}^{jk} = (\vec{\rho} \times \vec{r})^2\ [T_{jk}(\rho,\rho)-T_{jk}(r,r)] \sum_i a_i^{(7)}\ \frac{1}{\sqrt{385}} \times \frac{(2\lambda_i^{(7)})^{9/2}}{\pi^{3/2}}\ e^{-\lambda_i^{(7)}(\rho^2+r^2)}$$

$$\psi_8 = (\vec{\rho} \times \vec{r})^6 \sum_i a_i^{(8)} \frac{2}{45\sqrt{3 \times 7 \times 11 \times 13}}$$

$$\times \frac{(2\lambda_i^{(8)})^{15/2}}{\pi^{3/2}} e^{-\lambda_i^{(8)}(\rho^2+r^2)} \qquad [3] \quad S$$

$$\psi_{9a} = (\vec{\rho} \times \vec{r})^2\, 2(\vec{\rho}\cdot\vec{r}) \sum_i a_i^{(9)} \frac{1}{\sqrt{105}}$$

$$\times \frac{(2\lambda_i^{(9)})^{9/2}}{\pi^{3/2}} e^{-\lambda_i^{(9)}(\rho^2+r^2)}$$

$$[21] \quad S'$$

$$\psi_{9s} = (\vec{\rho} \times \vec{r})^2 (\rho^2-r^2) \sum_i a_i^{(9)} \frac{1}{\sqrt{105}}$$

$$\times \frac{(2\lambda_i^{(9)})^{9/2}}{\pi^{3/2}} e^{-\lambda_i^{(9)}(\rho^2+r^2)}$$

$$\psi_{10} = (\rho^2+r^2) \sum_i a_i^{(10)} \frac{(2\lambda_i^{(10)})^{5/2}}{\pi^{3/2}}$$

$$\times e^{-\lambda_i^{(10)}(\rho^2+r^2)} \qquad [3] \quad S$$

The j superscript of ψ_3^j refers to a component of the Cartesian vector, and jk in ψ_{4a}^{jk}, ψ_{4s}^{jk}, ψ_{7a}^{jk}, ψ_{7s}^{jk} refer to the cartesian components of the irreducible traceless symmetric tensors, i.e. j,k= 1, 2, or 3. The $a_i^{(s)}$ are the linear and the $\lambda_i^{(s)}$ are the non-linear parameters.

When we are finding the matrix elements of V_{12} with these wave functions, it is evident that for potentials that are repulsive near the origin, wave functions which include a factor ρ^n, $n \geqslant 1$ need to be used to ensure that the wave function is small near the origin. One could hope, of course, that the coefficients a_i in the sums would cause the wave function to vanish when $\rho = o$, but this will not happen for all r unless all $a_i^{(s)}$'s are zero. Thus for attractive potentials, we could use all of the states, but for potentials which have short range repulsion we would expect only ψ_3, ψ_5, ψ_6, ψ_7, ψ_8, ψ_9 to make the greatest contribution in the variational calculation. It is also to be expected that because of the centrifugal barrier, the D-state would favour functions that vanish as ρ tends to zero. Thus, even for attractive potentials, ψ_7 may be a better D-state than ψ_4.

If we consider only one term in each of the S-states, ψ_1, ψ_{10}, ψ_5, we have $e^{-\lambda(\rho^2+r^2)}$, $(\rho^2+r^2)e^{-\lambda(\rho^2+r^2)}$, and $(\vec{\rho} \times \vec{r})^2 e^{-\lambda(\rho^2+r^2)}$. It can be shown that these three states are linear combinations of the three lowest states in the six-dimensional harmonic oscillator (see Appendix A) with an oscillator constant of 2λ. Our trial functions, therefore, are basically the lowest states of the six-dimensional harmonic oscillator with different oscillator constants. Even though functions of the type $e^{-\lambda(\rho^2+r^2)}$ for differing λ do not form a complete set, we know that the set of oscillator functions is complete. Since the triton is a low energy system, we feel that the lowest energy oscillator functions with several different oscillator parameters mixed in in a variationally favourable way will give reasonable results.

The space wave function must be combined with the proper spin-isospin function to give an overall wave function that is totally antisymmetric with angular momentum $J=1/2$. We make use of the spin-isospin functions defined in Chapter II and obtain the following components of the total wave function.

$$\Psi_1 = \Gamma_1 \psi_1$$

$$\Psi_2 = \Gamma_{2a} \psi_{2s} - \Gamma_{2s} \psi_{2a}$$

$$\Psi_3 = \Gamma_3^{\,i} \psi_3^{\,i}$$

$$\Psi_4 = \Gamma_{4a}^{\,ij} \psi_{4s}^{\,ij} - \Gamma_{4s}^{\,ij} \psi_{4a}^{\,ij}$$

$$\Psi_5 = \Gamma_1 \psi_5$$

$$\Psi_6 = \Gamma_1 \psi_6$$

$$\Psi_7 = \Gamma_{4a}^{\,ij} \psi_{7s}^{\,ij} - \Gamma_{4s}^{\,ij} \psi_{7a}^{\,ij}$$

$$\Psi_8 = \Gamma_1 \psi_8$$

$$\Psi_9 = \Gamma_{2a} \psi_{9s} - \Gamma_{2s} \psi_{9a}$$

$$\Psi_{10} = \Gamma_1 \psi_{10}$$

The Γ_i can be obtained with the help of the angular isospin functions found in Table II-1.

$$\Gamma_1 = Y_1$$

$$\Gamma_{2a} = Y_{3,a}$$

$$\Gamma_{2s} = Y_{3,s}$$

$\Gamma_3{}^i$ is obtained from Y_4, and $\Gamma_{4a}{}^{ij}$ and $\Gamma_{4s}{}^{ij}$ are obtained from Y_8.

$$\Gamma_3{}^i = \frac{1}{\sqrt{2}} [\phi_i{}^{(1/2)}([21], a)\chi([21], a) + \phi_i{}^{(1/2)}([21], s)\chi([21], s)]$$

$$\Gamma_{4a}{}^{ij} = \phi_{ij}{}^{(3/2)}([3])\chi([21], a)$$

$$\Gamma_{4s}{}^{ij} = \phi_{ij}{}^{(3/2)}([3])\chi([21], s)$$

It is convenient to write $\Psi_i = \sum_j a_j{}^{(i)} \phi_j{}^{(i)}$ (no sum over i). The $\phi_j{}^{(i)}$'s are easily determined from the above expressions and the definitions of ψ_i. The total wave function is $\Psi = \sum_{i=1}^{10} \Psi_i$.

(ii) Normalization Matrix

The most straightforward matrix elements to calculate are the normalization matrix elements. Let us define a_i, λ_i, and ϕ_i with only one subscript and no superscripts such that i runs from 1, ..., N where N is the total number of linear and consequently also the number of non-linear parameters. Then $N = \sum_{i=1}^{10} n_i$ where n_i is the number of terms in Ψ_i. The normalization matrix elements are defined as $N_{ij} = \langle\phi_i|\phi_j\rangle$. In order to be able to calculate $\langle\phi_i|\phi_j\rangle$ we must make use of the orthogonality of the spin-isospin functions. That is

$$\langle\Gamma_i|\Gamma_j\rangle = 0 \quad \text{when } i \neq j$$

$$\langle\Gamma_1|\Gamma_1\rangle = \langle\Gamma_{2a}|\Gamma_{2a}\rangle = \langle\Gamma_{2s}|\Gamma_{2s}\rangle = 1$$

$$\langle\Gamma_{3i}|\Gamma_{3j}\rangle = \delta_{ij}$$

$$\langle\Gamma_{4a}{}^{ij}|\Gamma_{4a}{}^{k\ell}\rangle = \langle\Gamma_{4s}{}^{ij}|\Gamma_{4s}{}^{k\ell}\rangle = \delta_{ik}\,\delta_{j\ell}$$

The last expression is true only when Γ^{ij} is contracted with a traceless symmetric tensor, which is always the case in this work.

We calculate the normalization matrix elements between all possible states.

$$\langle\Psi_1|\Psi_1\rangle = \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^3$$

$$\langle\Psi_1|\Psi_5\rangle = \frac{3}{2}\,\frac{\lambda_j}{\lambda_i}\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^5$$

$$\langle\Psi_1|\Psi_6\rangle = \frac{\sqrt{70}}{42}\,\frac{\lambda_j^{\,2}}{\lambda_i^{\,2}}\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^7$$

$$\langle\Psi_1|\Psi_8\rangle = \frac{7}{2\sqrt{3 \times 7 \times 11 \times 13}}\,\frac{\lambda_j^{\,3}}{\lambda_i^{\,3}}\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^9$$

$$<\Psi_6|\Psi_8> = \frac{\sqrt{110}}{2\sqrt{39}} \frac{\lambda_j}{\lambda_i} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{13}$$

$$<\Psi_6|\Psi_{10}> = \frac{\sqrt{70}}{3} \frac{\lambda_i^{\,2}}{\lambda_j(\lambda_i + \lambda_j)} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{7}$$

$$<\Psi_7|\Psi_7> = \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{9}$$

$$<\Psi_8|\Psi_8> = \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{15}$$

$$<\Psi_8|\Psi_{10}> = \frac{63}{\sqrt{3 \times 7 \times 11 \times 13}} \frac{\lambda_i^{\,3}}{\lambda_j^{\,2}(\lambda_i + \lambda_j)} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{9}$$

$$<\Psi_9|\Psi_9> = \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{9}$$

$$<\Psi_{10}|\Psi_{10}> = 12 \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{5}$$

$<\Psi_s|\Psi_t> = <\Psi_t|\Psi_s>$ and all other possible combinations are zero.

It is now obvious why we chose to insert factors like $\frac{(2\lambda_i)^{5/2}}{\pi^{3/2}}$ in the trial wave function. In the normalization matrix elements, we obtain factors like $\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{5}$ which for i=j reduce to 1 regardless of the magnitude of the exponent. This same scaling factor ensures that all the matrix elements are of the same order of magnitude provided the λ_i's do not differ by more than an order of magnitude. In our calculations, we find that the greatest difference between the smallest and largest parameter is about a factor of ten. Having the matrix elements all of comparable size avoids trouble when one does matrix algebra.

It would have been possible to define the Ψ_i so that they were all orthogonal to each other. This would have had the advantage that the resultant normalization matrix would have block matrices along the diagonal only. But besides being able to evaluate each state's amplitude in the total wave function, it is of no advantage but rather it makes the analysis more cumbersome. We have to find the inverse of a non-singular matrix anyway, and since we do this numerically a few non-zero matrix elements more or less do not matter.

(iii) Kinetic Energy Matrix

The kinetic energy operator is given by $-\frac{\hbar^2}{2M}$ K where $K \equiv \nabla_{r_1}^{\;2} + \nabla_{r_2}^{\;2} + \nabla_{r_3}^{\;2} = \nabla_r^{\;2} + \nabla_\rho^{\;2}$ when operating on a function independent of the coordinates of the center-of-mass. M is the nucleon mass. Since K is a scalar operator and totally symmetric under interchange of space coordinates, it follows that only those matrix elements of kinetic energy are non-zero which correspond to non-zero matrix elements in the normalization matrix. When we calculate the effect of K on one term in each of the space functions we obtain the following expressions:

$$K\ e^{-\lambda(\rho^2+r^2)} = 4\lambda[-3 + \lambda(\rho^2+r^2)]\ e^{-\lambda(\rho^2+r^2)}$$

$$K\ 2(\vec{\rho}\cdot\vec{r})\ e^{-\lambda(\rho^2+r^2)} = 4\lambda[-5 + \lambda(\rho^2+r^2)]\ 2(\vec{\rho}\cdot\vec{r})\ e^{-\lambda(\rho^2+r^2)}$$

$$K\ (\rho^2-r^2)\ e^{-\lambda(\rho^2+r^2)} = 4\lambda[-5 + \lambda(\rho^2+r^2)](\rho^2-r^2)\ e^{-\lambda(\rho^2+r^2)}$$

$$K\ (\vec{\rho}\times\vec{r})_i\ e^{-\lambda(\rho^2+r^2)} = 4\lambda[-5 + \lambda(\rho^2+r^2)](\vec{\rho}\times\vec{r})_i\ e^{-\lambda(\rho^2+r^2)}$$

$$K\ 2T_{ij}(\rho,r)\ e^{-\lambda(\rho^2+r^2)} = 4\lambda[-5 + \lambda(\rho^2+r^2)]$$

$$\times\ 2T_{ij}(\rho,r)\ e^{-\lambda(\rho^2+r^2)}$$

$$K\ [T_{ij}(\rho,\rho) - T_{ij}(r,r)]\ e^{-\lambda(\rho^2+r^2)} = 4\lambda[-5 + \lambda(\rho^2+r^2)]$$

$$\times\ [T_{ij}(\rho,\rho) - T_{ij}(r,r)]\ e^{-\lambda(\rho^2+r^2)}$$

$$K\ (\vec{\rho}\times\vec{r})^2\ e^{-\lambda(\rho^2+r^2)} = \{4(\rho^2+r^2) + 4\lambda[-7 + \lambda(\rho^2+r^2)](\vec{\rho}\times\vec{r})^2\}$$

$$\times\ e^{-\lambda(\rho^2+r^2)}$$

$$K\ (\vec{\rho}\times\vec{r})^4\ e^{-\lambda(\rho^2+r^2)} = \{16(\rho^2+r^2)(\vec{\rho}\times\vec{r})^2$$

$$+ 4\lambda[-11 + \lambda(\rho^2+r^2)](\vec{\rho}\times\vec{r})^4\}e^{-\lambda(\rho^2+r^2)}$$

$$K\ (\vec{\rho}\times\vec{r})^2\ 2T_{ij}(\rho,r)\ e^{-\lambda(\rho^2+r^2)} = \{8(\rho^2+r^2)\ 2T_{ij}(\rho,r)$$

$$- 8(\vec{\rho}\cdot\vec{r})[T_{ij}(\rho,\rho) + T_{ij}(r,r)]$$

$$-36\lambda(\rho \times r)^2 \; 2T_{ij}(\rho,r)$$

$$+ 4\lambda^2(\rho^2+r^2)(\vec{\rho} \times \vec{r})^2 \; 2T_{ij}\;(\rho,r)\}$$

$$\times \; e^{-\lambda(\rho^2+r^2)}$$

$$K\;(\vec{\rho} \times \vec{r})^2 \;[T_{ij}(\rho,\rho) - T_{ij}(r,r)]\; e^{-\lambda(\rho^2+r^2)}$$

$$= \{4T_{ij}(\rho,\rho)(\rho^2+3r^2) - 4T_{ij}(r,r)(3\rho^2+r^2)$$

$$- 36\lambda(\vec{\rho} \times \vec{r})^2 \times [T_{ij}(\rho,\rho) - T_{ij}(r,r)]$$

$$+ 4\lambda^2(\rho^2+r^2)(\vec{\rho} \times \vec{r})^2 \;[T_{ij}(\rho,\rho)$$

$$- T_{ij}(r,r)]\}\; e^{-\lambda(\rho^2+r^2)}$$

$$K\;(\vec{\rho} \times \vec{r})^6 \; e^{-\lambda(\rho^2+r^2)} = \{36(\rho^2+r^2)(\vec{\rho} \times \vec{r})^4$$

$$+ 4\lambda[-15 + \lambda(\rho^2+r^2)](\vec{\rho} \times \vec{r})^6\}\; e^{-\lambda(\rho^2+r^2)}$$

$$K\;(\vec{\rho} \times \vec{r})^2 \; 2(\vec{\rho}\cdot\vec{r})\; e^{-\lambda(\rho^2+r^2)} = 8[(\rho^2+r^2)(\vec{\rho}\cdot\vec{r})$$

$$- 9\lambda(\vec{\rho} \times \vec{r})^2(\vec{\rho}\cdot\vec{r}) + \lambda^2(\rho^2+r^2)(\vec{\rho} \times \vec{r})^2(\vec{\rho}\cdot\vec{r})]$$

$$\times \; e^{-\lambda(\rho^2+r^2)}$$

$$K\;(\vec{\rho} \times \vec{r})^2(\rho^2-r^2)\; e^{-\lambda(\rho^2+r^2)} = 4[(\rho^2+r^2)(\rho^2-r^2)$$

$$- 9\lambda(\vec{\rho} \times \vec{r})^2(\rho^2-r^2) + \lambda^2(\rho^2+r^2)(\vec{\rho} \times \vec{r})^2(\rho^2-r^2)]$$

$$\times \; e^{-\lambda(\rho^2+r^2)}$$

$$\begin{aligned} K\,(\rho^2+r^2)\,e^{-\lambda(\rho^2+r^2)} &= 4[3 - 5\lambda(\rho^2+r^2) \\ &\quad + \lambda^2(\rho^4 + 2\rho^2 r^2 + r^4)]\,e^{-\lambda(\rho^2+r^2)} \end{aligned}$$

A useful relation that gives kinetic energy operator acting on states of the type $(\vec{\rho} \times \vec{r})^{2n}\,e^{-\lambda(\rho^2+r^2)}$ is

$$\begin{aligned} K\,(\vec{\rho} \times \vec{r})^{2n}\,e^{-\lambda(\rho^2+r^2)} &= \{4n^2(\rho^2+r^2)(\vec{\rho} \times \vec{r})^{2n-2} \\ &\quad + 4\lambda[-(3 + 4n) + \lambda(\rho^2+r^2)] \\ &\quad \times (\vec{\rho} \times \vec{r})^{2n}\}\,e^{-\lambda(\rho^2+r^2)} \end{aligned}$$

Because of the nature of the trial functions, it turns out that the kinetic energy matrix elements can be evaluated explicitly. Thus contracting the above expressions with the appropriate functions and inserting the scaling factors we obtain:

$$<\Psi_1|K|\Psi_1> = -3(\lambda_i+\lambda_j)\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^5$$

$$<\Psi_1|K|\Psi_5> = (\lambda_i + \lambda_j)\left(-\frac{9}{2}\frac{\lambda_j}{\lambda_i} + 3\right)\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^7$$

$$<\Psi_1|K|\Psi_6> = \frac{\sqrt{70}}{42}\,(\lambda_i + \lambda_j)\left(4-3\,\frac{\lambda_j}{\lambda_i}\right)\frac{\lambda_j}{\lambda_i}\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^9$$

$$<\Psi_1|K|\Psi_8> = \frac{21}{2\sqrt{3 \times 7 \times 11 \times 13}}\,(\lambda_i+\lambda_j)\left(2-\frac{\lambda_j}{\lambda_i}\right)\frac{\lambda_j^{\,2}}{\lambda_i^{\,2}}\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{11}$$

$$<\Psi_1|K|\Psi_{10}> = 6(\lambda_i - 3\lambda_j) \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^5$$

$$<\Psi_2|K|\Psi_2> = -30(\lambda_i + \lambda_j) \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^7$$

$$<\Psi_2|K|\Psi_9> = \frac{15}{\sqrt{105}} (\lambda_i + \lambda_j)(2-5 \frac{\lambda_j}{\lambda_i}) \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^9$$

$$<\Psi_3|K|\Psi_3> = - \frac{15}{2} (\lambda_i + \lambda_j) \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^7$$

$$<\Psi_4|K|\Psi_4> = -50 (\lambda_i + \lambda_j) \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^7$$

$$<\Psi_4|K|\Psi_7> = \frac{40}{\sqrt{385}} (\lambda_i + \lambda_j)(2-5 \frac{\lambda_j}{\lambda_i}) \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^9$$

$$<\Psi_5|K|\Psi_5> = \frac{15}{2} (\lambda_i + \lambda_j) \left[\frac{(\lambda_i+\lambda_j)^2}{\lambda_i\lambda_j} - 7\right] \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^9$$

$$<\Psi_5|K|\Psi_6> = \frac{\sqrt{70}}{12} (\lambda_i + \lambda_j)(8 - \frac{\lambda_j}{\lambda_i})(1-2 \frac{\lambda_j}{\lambda_i}) \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{11}$$

$$<\Psi_5|K|\Psi_8> = \frac{126}{\sqrt{3 \times 7 \times 11 \times 13}} (9\lambda_i^2 - 12\lambda_i\lambda_j + \lambda_j^2)$$

$$\frac{1}{\lambda_i + \lambda_j} \frac{\lambda_j^2}{\lambda_i^2} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{11}$$

$$\langle\Psi_5|K|\Psi_{10}\rangle = 3(3\lambda_i^{\,2} - 19\lambda_i\lambda_j + 8\lambda_j^{\,2})\ \frac{1}{\lambda_j}\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^7$$

$$\langle\Psi_6|K|\Psi_6\rangle = (\lambda_i + \lambda_j)\left[2\ \frac{(\lambda_i+\lambda_j)^2}{\lambda_i\lambda_j} - 11\right]\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{13}$$

$$\langle\Psi_6|K|\Psi_8\rangle = \frac{22\sqrt{10}}{5\sqrt{3 \times 11 \times 13}}\ (18\lambda_i^{\,2} - 39\lambda_i\lambda_j + 8\lambda_j^{\,2})$$

$$\frac{1}{\lambda_i + \lambda_j}\ \frac{\lambda_j}{\lambda_i}\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{13}$$

$$\langle\Psi_6|K|\Psi_{10}\rangle = \frac{\sqrt{70}}{21}\ (3\lambda_i^{\,2} - 29\lambda_i\lambda_j + 24\lambda_j^{\,2})\frac{\lambda_i}{\lambda_j^{\,2}}\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^9$$

$$\langle\Psi_7|K|\Psi_7\rangle = \left[\frac{56}{11}\ (\lambda_i + \lambda_j) - 36\ \frac{\lambda_i\lambda_j}{\lambda_i + \lambda_j}\right]\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^9$$

$$\langle\Psi_8|K|\Psi_8\rangle = 12(\lambda_i + \lambda_j)\left[1-5\ \frac{\lambda_i\lambda_j}{(\lambda_i+\lambda_j)^2}\right]\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{15}$$

$$\langle\Psi_8|K|\Psi_{10}\rangle = \frac{21}{\sqrt{3 \times 7 \times 11 \times 13}}\ (\lambda_i^{\,2} - 13\lambda_i\lambda_j + 16\lambda_j^{\,2})$$

$$\frac{\lambda_i^{\,2}}{\lambda_j^{\,3}}\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{11}$$

$$\langle\Psi_9|K|\Psi_9\rangle = 4(\lambda_i + \lambda_j)\left[1-9\ \frac{\lambda_i\lambda_j}{(\lambda_i+\lambda_j)^2}\right]\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^9$$

$$<\Psi_{10}|K|\Psi_{10}> = 12(3\lambda_i^{\,2} - 14\lambda_i\lambda_j + 3\lambda_j^{\,2}) \frac{1}{\lambda_i+\lambda_j} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^5$$

$<\Psi_t|K|\Psi_s> = <\Psi_s|K|\Psi_t>$ and all other possible matrix elements are zero.

(iv) Potential Energy Matrix

The Reid potential has a different analytic form for each different LSJ state where S is the two-body spin, L the two-body relative orbital angular momentum, J the two-body total angular momentum. For this reason, we would like to project out of the wave function those parts which have L, S, J as good quantum numbers. This is done by inspection. If we omit the factors

$\sum_j a_j^{(i)} \frac{(\lambda_j^{(i)})^{\frac{2n+1}{2}}}{\pi^{3/2}} \quad e^{-\lambda_j^{(i)}(\rho^2+r^2)}$, the trial wave functions can be written as

$$\Psi_1 = \frac{1}{\sqrt{2}}\,\phi\,\chi_s + \frac{1}{\sqrt{6}}\,(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})\phi\chi_a$$

$$\Psi_2 = \frac{1}{\sqrt{2}}\,(\rho^2-r^2)\phi\chi_s - \frac{1}{\sqrt{6}}\,(\rho^2-r^2)(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})\phi\chi_a$$

$$- \frac{2}{\sqrt{2}}\,(\vec{\rho}\cdot\vec{r})\phi\chi_a - \frac{2}{\sqrt{6}}\,(\vec{\rho}\cdot\vec{r})(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})\phi\chi_s$$

$$\Psi_3 = \frac{i}{\sqrt{2}}\,\vec{\rho}\cdot(\vec{r}\times\vec{\sigma}^{(3)})\phi\chi_a + \frac{i}{\sqrt{6}}\,(\vec{\rho}\times\vec{\sigma}^{(1)})\cdot\vec{r}\phi\chi_s$$

$$- \frac{1}{\sqrt{6}}\,(\vec{\rho}\cdot\vec{\sigma}^{(1)})(\vec{r}\cdot\vec{\sigma}^{(3)})\phi\chi_s + \frac{1}{\sqrt{6}}\,(\vec{\rho}\cdot\vec{\sigma}^{(3)})(\vec{r}\cdot\vec{\sigma}^{(1)})\phi\chi_s$$

$$\Psi_4 = [(\vec{\rho}\cdot\vec{\sigma}^{(1)})(\vec{\rho}\cdot\vec{\sigma}^{(3)}) - \frac{1}{3}\rho^2(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)}) - (\vec{r}\cdot\vec{\sigma}^{(1)})(\vec{r}\cdot\vec{\sigma}^{(3)})$$

$$+ \frac{1}{3} r^2(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})]\phi\chi_a - [(\vec{\rho}\cdot\vec{\sigma}^{(1)}(\vec{r}\cdot\vec{\sigma}^{(3)})$$

$$+ (\vec{\rho}\cdot\vec{\sigma}^{(3)})(\vec{r}\cdot\vec{\sigma}^{(1)}) - \frac{2}{3}(\vec{\rho}\cdot\vec{r})(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})]\phi\chi_s$$

$$\Psi_5 = \frac{1}{\sqrt{2}}[\rho^2 r^2 - (\vec{\rho}\cdot\vec{r})^2]\phi\chi_s + \frac{1}{\sqrt{6}}[\rho^2 r^2(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})$$

$$- (\vec{\rho}\cdot\vec{r})^2(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})]\phi\chi_a$$

$$\Psi_6 = \frac{1}{\sqrt{2}}[\rho^4 r^4 - 2\rho^2 r^2(\vec{\rho}\cdot\vec{r})^2 + (\vec{\rho}\cdot\vec{r})^4]\phi\chi_s$$

$$+ \frac{1}{\sqrt{6}}[\rho^4 r^4(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)}) - 2\rho^2 r^2(\vec{\rho}\cdot\vec{r})^2(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})$$

$$+ (\vec{\rho}\cdot\vec{r})^4(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})]\phi\chi_a$$

$$\Psi_7 = [\rho^2 r^2(\vec{\rho}\cdot\vec{\sigma}^{(1)})(\vec{\rho}\cdot\vec{\sigma}^{(3)}) - (\vec{\rho}\cdot\vec{r})^2(\vec{\rho}\cdot\vec{\sigma}^{(1)})(\vec{\rho}\cdot\vec{\sigma}^{(3)})$$

$$- \frac{1}{3}\rho^4 r^2(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)}) + \frac{1}{3}\rho^2(\vec{\rho}\cdot\vec{r})^2(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})$$

$$- \rho^2 r^2(\vec{r}\cdot\vec{\sigma}^{(1)})(\vec{r}\cdot\vec{\sigma}^{(3)}) + (\vec{\rho}\cdot\vec{r})^2(\vec{r}\cdot\vec{\sigma}^{(1)})(\vec{r}\cdot\vec{\sigma}^{(3)})$$

$$+ \frac{1}{3}\rho^2 r^4(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)}) - \frac{1}{3} r^2(\vec{\rho}\cdot\vec{r})^2(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})]\phi\chi_a$$

$$- [\rho^2 r^2(\vec{\rho}\cdot\vec{\sigma}^{(1)})(\vec{r}\cdot\vec{\sigma}^{(3)}) - (\vec{\rho}\cdot\vec{r})^2(\vec{\rho}\cdot\vec{\sigma}^{(1)})(\vec{r}\cdot\vec{\sigma}^{(3)})$$

$$+ \rho^2 r^2 (\vec{\rho}\cdot\vec{\sigma}^{(3)})(\vec{r}\cdot\vec{\sigma}^{(1)}) - (\vec{\rho}\cdot\vec{r})^2 (\vec{\rho}\cdot\vec{\sigma}^{(3)})(\vec{r}\cdot\vec{\sigma}^{(1)})$$

$$- \frac{2}{3} \rho^2 r^2 (\vec{\rho}\cdot\vec{r})(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)}) + \frac{2}{3} (\vec{\rho}\cdot\vec{r})^3 (\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})]\phi\chi_s$$

$$\Psi_8 = \frac{1}{\sqrt{2}} [\rho^6 r^6 - 3\rho^2 r^2 (\vec{\rho}\cdot\vec{r})^4 + 3\rho^4 r^4 (\vec{\rho}\cdot\vec{r})^2 - (\vec{\rho}\cdot\vec{r})^6]\phi\chi_s$$

$$+ \frac{1}{\sqrt{6}} [\rho^6 r^6 (\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)}) - 3\rho^2 r^2 (\vec{\rho}\cdot\vec{r})^4 (\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})$$

$$+ 3\rho^4 r^4 (\vec{\rho}\cdot\vec{r})^2 (\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)}) - (\vec{\rho}\cdot\vec{r})^6 (\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})]\phi\chi_a$$

$$\Psi_9 = \frac{1}{\sqrt{2}} (\rho^2 - r^2)[\rho^2 r^2 - (\vec{\rho}\cdot\vec{r})^2]\phi\chi_s$$

$$- \frac{1}{\sqrt{6}} (\rho^2 - r^2)[\rho^2 r^2 (\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)}) - (\vec{\rho}\cdot\vec{r})^2 (\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})]\phi\chi_a$$

$$- \frac{2}{\sqrt{2}} [\rho^2 r^2 (\vec{\rho}\cdot\vec{r}) - (\vec{\rho}\cdot\vec{r})^3]\phi\chi_a - \frac{2}{\sqrt{6}} [\rho^2 r^2 (\vec{\rho}\cdot\vec{r})(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})$$

$$- (\vec{\rho}\cdot\vec{r})^3 (\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})]\phi\chi_s$$

$$\Psi_{10} = \frac{1}{\sqrt{2}} (\rho^2 + r^2)\phi\chi_s + \frac{1}{\sqrt{6}} (\rho^2 + r^2)(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})\phi\chi_a .$$

We have used the short forms χ_s and χ_a to denote $\chi([21], s)$ and $\chi([21], a)$.

The spatial dependence of the wave functions is given in terms of the vectors $\vec{\rho}$ and $\vec{r}$. The vector $\vec{\rho}$ is proportional to the vector between particles one and two. This is to our advantage because we have to determine only the matrix element of V_{12}, since because of the antisymmetry of the overall wave function $\langle\Psi|V_{12}|\Psi\rangle = \langle\Psi|V_{13}|\Psi\rangle = \langle\Psi|V_{23}|\Psi\rangle$.

To decompose the wave function into the proper two-body orbital angular momentum components, we write the wave function as a sum of terms containing factors of the type 1, ρ^2, ρ_i, $T_{ij}(\rho,\rho)$, $T_{ijk}(\rho,\rho,\rho)$, ... These terms correspond to two-body S-, S-, P-, D-, F-,... states, respectively. Furthermore, we can get the proper spin-dependence by noting whether $\vec{\sigma}^{(1)}$ operates on ϕ or not. Since ϕ contains the antisymmetric two-body spin function ϕ_o i.e.

$$\phi = \frac{1}{\sqrt{2}} (\alpha_1\beta_2 - \alpha_2\beta_1)\alpha_3$$

$$\phi = \phi_o\alpha_3 ,$$

the operators $\vec{\sigma}^{(1)}$ and $\vec{\sigma}^{(2)}$ are linearly dependent when acting on ϕ, i.e.

$$\vec{\sigma}^{(1)}\phi_o = -\vec{\sigma}^{(2)}\phi_o$$

$$\text{thus} \qquad \vec{\sigma}^{(1)}\phi = -\vec{\sigma}^{(2)}\phi .$$

The state ϕ is a two-body spin singlet; the state $\sigma_i^{(1)}\phi$ is a two-body spin triplet. This can be seen from the transformational properties of $\sigma_i^{(1)}\phi$, i.e. it transforms like a vector. Combining the spatial factors with $\sigma_i^{(1)}$ if it is present, we obtain the two-body angular momentum by noting the overall two-body rotational properties, e.g. $\sigma_i^{(1)} T_{ijk}(\rho,\rho,\rho)$ gives J=2 since it transforms like an irreducible tensor of rank 2. The complete wave function must be a scalar and therefore such two-body components as described above must be contracted with traceless symmetric tensors formed from one vector operator $\vec{\sigma}^{(3)}$ and the vector $\vec{r}$ as many times as is necessary to obtain a tensor of the appropriate rank. By this procedure of finding all possible combinations for a particular three-body state, and determining their coefficients, we decompose Ψ_i into a sum of terms, $\Psi_i = \sum_j k_j$. The k_j's are given in Table III-1. We have indicated the two-body quantum numbers of each k_j and the angular momentum associated with the vector $\vec{r}$. The latter quantity is useful in determining the orthogonality of the various k_j's. The k_j's are not of definite three-body symmetry; it is, therefore, imperative that all the components, k_j, of any one Ψ_i are retained in the calculation in order to ensure overall antisymmetry.

At this point we can find out how the different states are connected. The Reid potential is given, and indeed any potential can be expressed, in such a way that the matrix elements between pure two-body LSJ states can be found. We can write down the integrals for the central part of the potential; this includes $\vec{L}\cdot\vec{S}$ or L^2 parts since they conserve LSJ. We have given these integrals in Table III-2. Whereas before we found that there were many zero elements in the normalization and kinetic energy matrices, for the potential energy matrix elements there are very few states not connected by the force.

To find the matrix elements of the tensor operator, we express this operator as a scalar product of two second rank tensors, $S_{12} = \frac{3}{\rho^2} T_{ij}(\rho,\rho) T_{ij}(\sigma^{(1)}, \sigma^{(2)})$. After doing some tensor arithmetic, we arrive at the matrix elements given in Table III-3. We find that the tensor operator couples the three-body S-state to the three-body D-state. The P-state is coupled to the three-body D-state also via the tensor force. The P-state is only coupled to the S-state in second order.

Now we are in a position to write down explicitly the matrix elements. Let us define the following integrals where V_i's are given in Table III-4.

$$A_i = \frac{\pi}{\lambda^{3/2}} \int e^{-\lambda\rho^2} V_i(\rho) d\vec{\rho}$$

$$B_i = \frac{\pi}{\lambda^{5/2}} \int \rho^2 e^{-\lambda\rho^2} V_i(\rho) d\vec{\rho}$$

$$C_i = \frac{\pi}{\lambda^{7/2}} \int \rho^4 e^{-\lambda\rho^2} V_i(\rho) d\vec{\rho}$$

$$D_i = \frac{\pi}{\lambda^{9/2}} \int \rho^6 e^{-\lambda\rho^2} V_i(\rho) d\vec{\rho}$$

$$E_i = \frac{\pi}{\lambda^{11/2}} \int \rho^8 e^{-\lambda\rho^2} V_i(\rho) d\vec{\rho}$$

$$F_i = \frac{\pi}{\lambda^{13/2}} \int \rho^{10} e^{-\lambda\rho^2} V_i(\rho) d\vec{\rho}$$

$$G_i = \frac{\pi}{\lambda^{15/2}} \int \rho^{12} e^{-\lambda\rho^2} V_i(\rho) d\vec{\rho}$$

We note that V_{13} and V_{21} are not pure J states but are the weighted averages. Since these are higher angular momenta states, the binding energy will not be very sensitive to them. The potential energy matrix elements are given in Table III-5. All the constants appearing in the expressions are exact.

(v) Root-mean-square Radius

The root-mean-square radius is given by $\sqrt{\langle R^2\rangle}$. $\langle R^2\rangle = \int \rho(r')r'^2 d\tau$ where r' is the distance of one of the three nucleons from the center-of-mass, and $\rho(r')$ is the probability density of the nucleon at r'. Because of the symmetry of the system only one nucleon needs to be considered. Otherwise, an integral like the above would have to be evaluated for all three particles and their sum divided by three. If the problem is expressed in terms of the interparticle distances, we obtain

$$R^2_{r.m.s.} = \int \psi_s \{\frac{1}{2}[2(r_1{}^2 + r_2{}^2) - r_3{}^2]\} \psi_s 8\pi^2 r_1 r_2 r_3 dr_1 dr_2 dr_3$$

for the totally symmetric S-state (L68).

In our formalism we can determine in general what the matrix elements are for the mean-square radius using ρ^2, r^2, and $(\vec{\rho}\cdot\vec{r})$ as coordinates. It is easy to show that

$$R^2 = \frac{1}{\sqrt{3}}(\vec{\rho}\cdot\vec{r}) + \frac{1}{2}\rho^2 + \frac{1}{6}r^2 .$$

The matrix elements would be

$$R^2_{r.m.s.} = \int \Psi_i \, [\frac{1}{\sqrt{3}}(\vec{\rho}\cdot\vec{r}) + \frac{1}{2}\rho^2 + \frac{1}{6}r^2]\Psi_j \, d\vec{r}d\vec{\rho}$$

Since the product $\Psi_i \Psi_j$ for i and j for which Ψ_i and Ψ_j are not spin-isospin orthogonal include only terms with even powers of $(\vec{\rho} \cdot \vec{r})$, the first term in the integral averages to zero. Hence effectively

$$R^2_{r.m.s.} = \int \Psi_i \left[\frac{1}{2}\rho^2 + \frac{1}{6} r^2\right] \Psi_j \, d\vec{r} d\vec{\rho} \ .$$

In table III-6 we list the matrix elements of the mean-square radius operator in terms of the normalization matrix elements. The simple expressions for this matrix are due to the fact that we have been using harmonic oscillator wave functions as our basis of functions.

TABLE III-1

		2-Particle State	$\vec{r}$-State
Ψ_1	$k_1 = \frac{1}{\sqrt{2}}\,\phi\chi_s$	^1S_o	S
	$k_2 = \frac{1}{\sqrt{6}}\,(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})\,\phi\chi_a$	$^3S_1$	S
Ψ_2	$k_3 = \frac{1}{\sqrt{2}}\,(\rho^2-r^2)\,\phi\chi_s$	^1S_o	S
	$k_4 = -\frac{1}{\sqrt{6}}\,(\rho^2-r^2)(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})\,\phi\chi_a$	$^3S_1$	S
	$k_5 = -\frac{2}{\sqrt{2}}\,(\vec{\rho}\cdot\vec{r})\,\phi\chi_a$	$^1P_1$	P
	$k_6 = -\frac{2}{3\sqrt{6}}\,(\vec{\rho}\cdot\vec{\sigma}^{(1)})(\vec{r}\cdot\vec{\sigma}^{(3)})\,\phi\chi_s$	^3P_o	P
	$k_7 = -\frac{1}{\sqrt{6}}\,(\vec{\rho} \times \vec{\sigma}^{(1)})\cdot(\vec{r} \times \vec{\sigma}^{(3)})\,\phi\chi_s$	$^3P_1$	P
	$k_8 = -\frac{2}{\sqrt{6}}\,T_{ij}(\rho,\sigma^{(1)})\,T_{ij}(r,\sigma^{(3)})\,\phi\chi_s$	$^3P_2$	P
Ψ_3	$k_9 = \frac{i}{\sqrt{2}}\,\vec{\rho}\cdot(\vec{r} \times \vec{\sigma}^{(3)})\,\phi\chi_a$	$^1P_1$	P
	$k_{10} = -\frac{2}{3\sqrt{6}}\,(\vec{\rho}\cdot\vec{\sigma}^{(1)})(\vec{r}\cdot\vec{\sigma}^{(3)})\,\phi\chi_s$	^3P_o	P
	$k_{11} = -\frac{1}{2\sqrt{6}}\,(\vec{\rho} \times \vec{\sigma}^{(1)})\cdot(\vec{r} \times \vec{\sigma}^{(3)})\,\phi\chi_s$	$^3P_1$	P
	$k_{12} = \frac{i}{\sqrt{6}}\,(\vec{\rho} \times \vec{\sigma}^{(1)})\cdot\vec{r}\,\phi\chi_s$	$^3P_1$	P
	$k_{13} = \frac{1}{\sqrt{6}}\,T_{ij}(\rho,\sigma^{(1)})\,T_{ij}(r,\sigma^{(3)})\,\phi\chi_s$	$^3P_2$	P

		2-Particle State	$\vec{r}$-State
Ψ_4	$k_{14} = - T_{ij}(r,r)\sigma_i^{(1)}\sigma_j^{(3)}\phi\chi_a$	$^3S_1$	D
	$k_{15} = T_{ij}(\rho,\rho)\sigma_i^{(1)}\sigma_j^{(3)}\phi\chi_a$	$^3D_1$	S
	$k_{16} = - \frac{10}{9}(\vec{\rho}\cdot\vec{\sigma}^{(1)})(\vec{r}\cdot\vec{\sigma}^{(3)})\phi\chi_s$	$^3P_0$	P
	$k_{17} = \frac{5}{6}(\vec{\rho} \times \vec{\sigma}^{(1)})\cdot(\vec{r} \times \vec{\sigma}^{(3)})\phi\chi_s$	$^3P_1$	P
	$k_{18} = - \frac{1}{3} T_{ij}(\rho,\sigma^{(1)})T_{ij}(r,\sigma^{(3)})\phi\chi_s$	$^3P_2$	P
Ψ_5	$k_{19} = \frac{2}{3\sqrt{2}}\rho^2 r^2 \phi\chi_s$	$^1S_0$	S
	$k_{20} = - \frac{1}{\sqrt{2}} T_{ij}(\rho,\rho)T_{ij}(r,r)\phi\chi_s$	$^1D_2$	D
	$k_{21} = \frac{2}{3\sqrt{6}}\rho^2 r^2(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})\phi\chi_a$	$^3S_1$	S
	$k_{22} = \frac{-3}{5\sqrt{6}} T_{ij}(\rho,\rho)T_{ik}(r,r)$ $\sigma_j^{(1)}\sigma_k^{(3)}\phi\chi_a$	$^3D_1$	D
	$k_{23} = - \frac{2}{3\sqrt{6}} T_{ij}(\rho,\rho \times \sigma^{(1)})$ $T_{ij}(r,r \times \sigma^{(3)})\phi\chi_a$	$^3D_2$	D
	$k_{24} = - \frac{1}{\sqrt{6}} T_{ijk}(\rho,\rho,\sigma^{(1)})$ $T_{ijk}(r,r,\sigma^{(3)})\phi\chi_a$	$^3D_3$	D
Ψ_6	$k_{25} = \frac{8}{15\sqrt{2}}\rho^4 r^4 \phi\chi_s$	$^1S_0$	S
	$k_{26} = \frac{-8}{7\sqrt{2}}\rho^2 r^2 T_{ij}(\rho,\rho)T_{ij}(r,r)\phi\chi_s$	$^1D_2$	D

	2-Particle State	$\vec{r}$-State
$k_{27} = \frac{1}{\sqrt{2}} T_{ijk\ell}(\rho,\rho,\rho,\rho)$ $T_{ijk\ell}(r,r,r,r,)\phi\chi_s$	$^1G_4$	G
$k_{28} = \frac{8}{15\sqrt{6}} \rho^4 r^4 (\vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(3)})\phi\chi_a$	$^3S_1$	S
$k_{29} = -\frac{24}{35\sqrt{6}} \rho^2 r^2\ T_{ij}(\rho,\rho)$ $T_{ik}(r,r)\sigma_j{}^{(1)}\sigma_k{}^{(3)}\phi\chi_a$	$^3D_1$	D
$k_{30} = -\frac{16}{21\sqrt{6}} \rho^2 r^2\ T_{ij}(\rho,\rho \times \sigma^{(1)})$ $T_{ij}(r,r \times \sigma^{(3)}\phi\chi_a$	$^3D_2$	D
$k_{31} = -\frac{8}{7\sqrt{6}} \rho^2 r^2\ T_{ijk}(\rho,\rho,\sigma^{(1)})$ $T_{ijk}(r,r,\sigma^{(3)})\phi\chi_a$	$^3D_3$	D
$k_{32} = \frac{7}{9\sqrt{6}} T_{ijk\ell}(\rho,\rho,\rho,\rho)T_{ijkm}(r,r,r,r)$ $\sigma_\ell{}^{(1)}\sigma_m{}^{(3)}\phi\chi_a$	$^3G_3$	G
$k_{33} = \frac{4}{5\sqrt{6}} T_{ijk\ell}(\rho,\rho,\rho,\rho \times \sigma^{(1)})$ $T_{ijk\ell}(r,r,r,r \times \sigma^{(3)})\phi\chi_a$	$^3G_4$	G
$k_{34} = \frac{1}{\sqrt{6}} T_{ijk\ell m}(\rho,\rho,\rho,\rho,\sigma^{(1)})$ $T_{ijk\ell m}(r,r,r,r,\sigma^{(3)})\phi\chi_a$	$^3G_5$	G
$k_{32,J} = \frac{1}{\sqrt{6}} T_{ijk\ell}(\rho,\rho,\rho,\rho)$ $T_{ijk\ell}(r,r,r,r)$ $(\vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(3)})\phi\chi_a$	^3G_J	G

		2-Particle State	r-State
Ψ_7	$k_{35} = -\frac{2}{3}(\rho^2 r^2 + \frac{1}{5}\rho^4)T_{ij}(r,r)$ $\sigma_i^{(1)}\sigma_j^{(3)}\phi\chi_a$	$^3S_1$	D
	$k_{36} = \frac{2}{3}(\rho^2 r^2 + \frac{1}{5}r^4)T_{ij}(\rho,\rho)$ $\sigma_i^{(1)}\sigma_j^{(3)}\phi\chi_a$	$^3D_1$	S
	$k_{37} = -\frac{1}{5}(\rho^2 - r^2)T_{ij}(\rho,\rho)T_{ik}(r,r)$ $\sigma_i^{(1)}\sigma_k^{(3)}\phi\chi_a$	$^3D_1$	D
	$k_{38} = \frac{2}{9}(\rho^2 - r^2)T_{ij}(\rho,\rho \times \sigma^{(1)})$ $T_{ij}(r,r \times \sigma^{(3)})\phi\chi_a$	$^3D_2$	D
	$k_{39} = -\frac{2}{21}(\rho^2 - r^2)T_{ijk}(\rho,\rho,\sigma^{(1)})$ $T_{ijk}(r,r,\sigma^{(3)})\phi\chi_a$	$^3D_3$	D
	$k_{40} = T_{ijk}(\rho,\rho,\sigma^{(1)})T_{ijk\ell}(r,r,r,r)$ $\sigma_\ell^{(3)}\phi\chi_a$	$^3D_3$	G
	$k_{41} = -T_{ijk\ell}(\rho,\rho,\rho,\rho)T_{ijk}(r,r,\sigma^{(3)})$ $\sigma_\ell^{(1)}\phi\chi_a$	$^3G_3$	D
	$k_{42} = -\frac{32}{45}\rho^2 r^2 (\vec{\rho}\cdot\vec{\sigma}^{(1)})(\vec{r}\cdot\vec{\sigma}^{(3)})\phi\chi_s$	^3P_o	P
	$k_{43} = \frac{8}{15}\rho^2 r^2 (\vec{\rho} \times \vec{\sigma}^{(1)})\cdot(\vec{r} \times \vec{\sigma}^{(3)})\phi\chi_s$	$^3P_1$	P
	$k_{44} = -\frac{16}{75}\rho^2 r^2 T_{ij}(\rho,\sigma^{(1)})$ $T_{ij}(r,\sigma^{(3)})\phi\chi_s$	$^3P_2$	P

		2-Particle State	$\vec{r}$-State
	$k_{45} = \frac{4}{5}\,\rho^2\, T_{ij}(\rho,\sigma^{(1)})$		
	$T_{ijk}(r,r,r)\sigma_k^{(3)}\phi\chi_s$	${}^3P_2$	F
	$k_{46} = \frac{4}{5}\,r^2\, T_{ijk}(\rho,\rho,\rho)$		
	$T_{ij}(r,\sigma^{(3)})\sigma_k^{(1)}\phi\chi_s$	${}^3F_2$	P
	$k_{47} = \frac{4}{7}\, T_{ijk}(\rho,\rho,\rho)$		
	$T_{ij\ell}(r,r,r)\sigma_k^{(1)}\sigma_\ell^{(3)}\phi\chi_s$	${}^3F_2$	F
	$k_{48} = -\frac{3}{4}\, T_{ijk}(\rho,\rho,\rho \times \sigma^{(1)})$		
	$T_{ijk}(r,r,r \times \sigma^{(3)})\phi\chi_s$	${}^3F_3$	F
	$k_{49} = \frac{1}{3}\, T_{ijk\ell}(\rho,\rho,\rho,\sigma^{(1)})$		
	$T_{ijk\ell}(r,r,r,\sigma^{(3)})\phi\chi_s$	${}^3F_4$	F
Ψ_8	$k_{50} = \frac{16}{35\sqrt{2}}\,\rho^6 r^6\, \phi\chi_s$	${}^1S_o$	S
	$k_{51} = -\frac{8}{7\sqrt{2}}\,\rho^4 r^4\, T_{ij}(\rho,\rho)T_{ij}(r,r)\phi\chi_s$	${}^1D_2$	D
	$k_{52} = \frac{18}{11\sqrt{2}}\,\rho^2 r^2\, T_{ijk\ell}(\rho,\rho,\rho,\rho)$		
	$T_{ijk\ell}(r,r,r,r)\phi\chi_s$	${}^1G_4$	G
	$k_{53} = \frac{16}{35\sqrt{6}}\,\rho^6 r^6 (\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})\phi\chi_a$	${}^3S_1$	S
	$k_{54} = -\frac{24}{35\sqrt{6}}\,\rho^4 r^4\, T_{ij}(\rho,\rho)T_{ik}(r,r)$		
	$\sigma_j^{(1)}\sigma_k^{(3)}\phi\chi_a$	${}^3D_1$	D

	2-Particle State	$\vec{r}$-State
$k_{55} = -\frac{16}{21\sqrt{6}} \rho^4 r^4 T_{ij}(\rho, \rho \times \sigma^{(1)})$ $T_{ij}(r, r \times \sigma^{(3)}) \phi \chi_a$	$^3D_2$	D
$k_{56} = -\frac{8}{7\sqrt{6}} \rho^4 r^4 T_{ijk}(\rho, \rho, \sigma^{(1)})$ $T_{ijk}(r, r, \sigma^{(3)}) \phi \chi_a$	$^3D_3$	D
$k_{57} = \frac{14}{11\sqrt{6}} \rho^2 r^2 T_{ijk\ell}(\rho, \rho, \rho, \rho)$ $T_{ijkm}(r, r, r, r) \sigma_\ell^{(1)} \sigma_m^{(3)} \phi \chi_a$	$^3G_3$	G
$k_{58} = \frac{72}{55\sqrt{6}} \rho^2 r^2 T_{ijk\ell}(\rho, \rho, \rho, \rho \times \sigma^{(1)})$ $T_{ijk\ell}(r, r, r, r \times \sigma^{(3)}) \phi \chi_a$	$^3G_4$	G
$k_{59} = \frac{18}{11\sqrt{6}} \rho^2 r^2 T_{ijk\ell m}(\rho, \rho, \rho, \rho, \sigma^{(1)})$ $T_{ijk\ell m}(r, r, r, r, \sigma^{(3)}) \phi \chi_a$	$^3G_5$	G
$k_{57,J} = \frac{18}{11\sqrt{6}} \rho^2 r^2 T_{ijk\ell}(\rho, \rho, \rho, \rho)$ $T_{ijk\ell}(r, r, r, r)$ $(\vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(3)}) \phi \chi_a$	^3G_J	G
$k_{60} = -\frac{1}{\sqrt{2}} T_{ijk\ell mn}(\rho, \rho, \rho, \rho, \rho, \rho)$ $T_{ijk\ell mn}(r, r, r, r, r, r) \phi \chi_s$	$^1I_6$	I

		2-Particle State	$\vec{r}$-State
	$k_{61,J} = -\frac{1}{\sqrt{6}} T_{ijk\ell mn}(\rho,\rho,\rho,\rho,\rho,\rho)\, T_{ijk\ell mn}(r,r,r,r,r,r)\, (\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})\phi\chi_a$	^3I_J	I
Ψ_9	$k_{64} = \frac{2}{3\sqrt{2}} (\rho^2-r^2)\rho^2 r^2\, \phi\chi_s$	^1S_o	S
	$k_{65} = -\frac{1}{\sqrt{2}} (\rho^2-r^2) T_{ij}(\rho,\rho) T_{ij}(r,r)\phi\chi_s$	$^1D_2$	D
	$k_{66} = -\frac{4}{5\sqrt{2}} \rho^2 r^2\, (\vec{\rho}\cdot\vec{r})\phi\chi_a$	$^1P_1$	P
	$k_{67} = \frac{2}{\sqrt{2}} T_{ijk}(\rho,\rho,\rho) T_{ijk}(r,r,r)\phi\chi_a$	$^1F_3$	F
	$k_{68} = -\frac{4}{15\sqrt{6}} \rho^2 r^2 (\vec{\rho}\cdot\vec{\sigma}^{(1)})(\vec{r}\cdot\vec{\sigma}^{(3)})\phi\chi_s$	^3P_o	P
	$k_{69} = -\frac{2}{5\sqrt{6}} \rho^2 r^2 (\vec{\rho} \times \vec{\sigma}^{(1)})\cdot(\vec{r}\times\vec{\sigma}^{(3)})\phi\chi_s$	$^3P_1$	P
	$k_{70} = -\frac{4}{5\sqrt{6}} \rho^2 r^2\, T_{ij}(\rho,\sigma^{(1)})\, T_{ij}(r,\sigma^{(3)})\phi\chi_s$	$^3P_2$	P
	$k_{71} = \frac{10}{7\sqrt{6}} T_{ijk}(\rho,\rho,\rho) T_{ij\ell}(r,r,r)\, \sigma_k^{(1)}\sigma_\ell^{(3)}\phi\chi_s$	$^3F_2$	F
	$k_{72} = \frac{3}{2\sqrt{6}} T_{ijk}(\rho,\rho,\rho \times \sigma^{(1)})\, T_{ijk}(r,r,r \times \sigma^{(3)})\phi\chi_s$	$^3F_3$	F
	$k_{73} = \frac{2}{\sqrt{6}} T_{ijk\ell}(\rho,\rho,\rho,\sigma^{(1)})\, T_{ijk\ell}(r,r,r,\sigma^{(3)})\phi\chi_s$	$^3F_4$	F

		2-Particle State	$\vec{r}$-State
	$k_{74} = -\frac{2}{3\sqrt{6}}(\rho^2-r^2)\rho^2r^2$ $(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})\phi\chi_a$	$^3S_1$	S
	$k_{75} = \frac{3}{5\sqrt{6}}(\rho^2-r^2)T_{ij}(\rho,\rho)$ $T_{ik}(r,r)\sigma_j^{(1)}\sigma_k^{(3)}\phi\chi_a$	$^3D_1$	D
	$k_{76} = \frac{2}{3\sqrt{6}}(\rho^2-r^2)T_{ij}(\rho,\rho \times \sigma^{(1)})$ $T_{ij}(r,r \times \sigma^{(3)})\phi\chi_a$	$^3D_2$	D
	$k_{77} = \frac{1}{\sqrt{6}}(\rho^2-r^2)T_{ijk}(\rho,\rho,\sigma^{(1)})$ $T_{ijk}(r,r,\sigma^{(3)})\phi\chi_a$	$^3D_3$	D
Ψ_{10}	$k_{78} = \frac{1}{\sqrt{2}}(\rho^2+r^2)\phi\chi_s$	^1S_o	S
	$k_{79} = \frac{1}{\sqrt{6}}(\rho^2+r^2)(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(3)})\phi\chi_a$	$^3S_1$	S

TABLE III-2

Diagonal Potential Energy Matrix Elements

Diagonal matrix elements exist when k_i and k_j both have the same two-body LSJ dependence. By $<k_i|k_j>$ we mean matrix elements of the potential in the state LSJ, i.e.

$$<k_i|k_j> \equiv <k_i(LSJ)|V_{12}|k_j(LSJ)> \equiv \int V(\rho)f(\rho^2,r^2)e^{-\lambda(\rho^2+r^2)}d\vec{r}d\vec{\rho}$$

where $\lambda = \lambda_i + \lambda_j$

and the isospin-angular momentum part is evaluated explicitly and included in $f(\rho^2,r^2)$. For notational convenience let us write

$$\int f(\rho^2,r^2) \equiv \int V(\rho)f(\rho^2,r^2)e^{-\lambda(\rho^2+r^2)}d\vec{r}d\vec{\rho}$$

After each matrix element we give the LSJ dependence and the three-body states in which k_i and k_j are found respectively.

$<k_1|k_1> = \frac{1}{2}\int 1$ $\quad {}^1S_o \quad \Psi_1 \quad \Psi_1$

$<k_2|k_2> = \frac{1}{2}\int 1$ $\quad {}^3S_1 \quad \Psi_1 \quad \Psi_1$

$<k_1|k_3> = \frac{1}{2}\int(\rho^2-r^2)$ $\quad {}^1S_o \quad \Psi_1 \quad \Psi_2$

$<k_2|k_4> = -\frac{1}{2}\int(\rho^2-r^2)$ $\quad {}^3S_1 \quad \Psi_1 \quad \Psi_2$

$\langle k_1|k_{19}\rangle = \frac{1}{3}\int \rho^2 r^2$ ${}^1S_o \quad \Psi_1 \quad \Psi_5$
$\langle k_2|k_{21}\rangle = \frac{1}{3}\int \rho^2 r^2$ ${}^3S_1 \quad \Psi_1 \quad \Psi_5$

$\langle k_1|k_{25}\rangle = \frac{4}{15}\int \rho^4 r^4$ ${}^1S_o \quad \Psi_1 \quad \Psi_6$
$\langle k_2|k_{28}\rangle = \frac{4}{15}\int \rho^4 r^4$ ${}^3S_1 \quad \Psi_1 \quad \Psi_6$

$\langle k_1|k_{50}\rangle = \frac{8}{35}\int \rho^6 r^6$ ${}^1S_o \quad \Psi_1 \quad \Psi_8$
$\langle k_2|k_{53}\rangle = \frac{8}{35}\int \rho^6 r^6$ ${}^3S_1 \quad \Psi_1 \quad \Psi_8$

$\langle k_1|k_{64}\rangle = \frac{1}{3}\int (\rho^4 r^2 - \rho^2 r^4)$ ${}^1S_o \quad \Psi_1 \quad \Psi_9$
$\langle k_2|k_{74}\rangle = -\frac{1}{3}\int (\rho^4 r^2 - \rho^2 r^4)$ ${}^3S_1 \quad \Psi_1 \quad \Psi_9$

$\langle k_1|k_{78}\rangle = \frac{1}{2}\int (\rho^2 + r^2)$ ${}^1S_o \quad \Psi_1 \quad \Psi_{10}$
$\langle k_2|k_{79}\rangle = \frac{1}{2}\int (\rho^2 + r^2)$ ${}^3S_1 \quad \Psi_1 \quad \Psi_{10}$

$\langle k_3|k_3\rangle = \frac{1}{2}\int (\rho^4 - 2\rho^2 r^2 + r^4)$ ${}^1S_o \quad \Psi_2 \quad \Psi_2$
$\langle k_4|k_4\rangle = \frac{1}{2}\int (\rho^4 - 2\rho^2 r^2 + r^4)$ ${}^3S_1 \quad \Psi_2 \quad \Psi_2$
$\langle k_5|k_5\rangle = \frac{2}{3}\int \rho^2 r^2$ ${}^1P_1 \quad \Psi_2 \quad \Psi_2$
$\langle k_6|k_6\rangle = \frac{2}{27}\int \rho^2 r^2$ ${}^3P_o \quad \Psi_2 \quad \Psi_2$

$\langle k_7|k_7\rangle = \frac{2}{9}\int \rho^2 r^2$ $\qquad {}^3P_1 \quad \Psi_2 \quad \Psi_2$

$\langle k_8|k_8\rangle = \frac{10}{27}\int \rho^2 r^2$ $\qquad {}^3P_2 \quad \Psi_2 \quad \Psi_2$

$\langle k_6|k_{10}\rangle = \frac{2}{27}\int \rho^2 r^2$ $\qquad {}^3P_o \quad \Psi_2 \quad \Psi_3$

$\langle k_7|k_{11}\rangle = \frac{1}{9}\int \rho^2 r^2$ $\qquad {}^3P_1 \quad \Psi_2 \quad \Psi_3$

$\langle k_8|k_{13}\rangle = -\frac{5}{27}\int \rho^2 r^2$ $\qquad {}^3P_2 \quad \Psi_2 \quad \Psi_3$

$\langle k_6|k_{16}\rangle = \frac{20}{27\sqrt{6}}\int \rho^2 r^2$ $\qquad {}^3P_o \quad \Psi_2 \quad \Psi_4$

$\langle k_7|k_{17}\rangle = -\frac{10}{9\sqrt{6}}\int \rho^2 r^2$ $\qquad {}^3P_1 \quad \Psi_2 \quad \Psi_4$

$\langle k_8|k_{18}\rangle = \frac{10}{27\sqrt{6}}\int \rho^2 r^2$ $\qquad {}^3P_2 \quad \Psi_2 \quad \Psi_4$

$\langle k_3|k_{19}\rangle = \frac{1}{3}\int (\rho^4 r^2 - \rho^2 r^4)$ $\qquad {}^1S_o \quad \Psi_2 \quad \Psi_5$

$\langle k_4|k_{21}\rangle = -\frac{1}{3}\int (\rho^4 r^2 - \rho^2 r^4)$ $\qquad {}^3S_1 \quad \Psi_2 \quad \Psi_5$

$\langle k_3|k_{25}\rangle = \frac{4}{15}\int (\rho^6 r^4 - \rho^4 r^6)$ $\qquad {}^1S_o \quad \Psi_2 \quad \Psi_6$

$\langle k_4|k_{28}\rangle = -\frac{4}{15}\int (\rho^6 r^4 - \rho^4 r^6)$ $\qquad {}^3S_1 \quad \Psi_2 \quad \Psi_6$

$\langle k_6|k_{42}\rangle = \frac{64}{135\sqrt{6}}\int \rho^4 r^4$ $\qquad {}^3P_o \quad \Psi_2 \quad \Psi_7$

$\langle k_7|k_{43}\rangle = -\frac{32}{45\sqrt{6}}\int \rho^4 r^4$ $\qquad {}^3P_1 \quad \Psi_2 \quad \Psi_7$

$\langle k_8|k_{44}\rangle = \frac{32}{135\sqrt{6}}\int \rho^4 r^4$ $\qquad {}^3P_2 \quad \Psi_2 \quad \Psi_7$

$$<k_3|k_{50}> = \frac{8}{35}\int(\rho^8 r^6 - \rho^6 r^8) \qquad {}^1S_o \quad \Psi_2 \quad \Psi_8$$

$$<k_4|k_{53}> = -\frac{8}{35}\int(\rho^8 r^6 - \rho^6 r^8) \qquad {}^3S_1 \quad \Psi_2 \quad \Psi_8$$

$$<k_3|k_{64}> = \frac{1}{3}\int(\rho^6 r^2 - 2\rho^4 r^4 + \rho^2 r^6) \qquad {}^1S_o \quad \Psi_2 \quad \Psi_9$$

$$<k_4|k_{74}> = \frac{1}{3}\int(\rho^6 r^2 - 2\rho^4 r^4 + \rho^3 r^6) \qquad {}^3S_1 \quad \Psi_2 \quad \Psi_9$$

$$<k_5|k_{66}> = \frac{4}{15}\int\rho^4 r^4 \qquad {}^1P_1 \quad \Psi_2 \quad \Psi_9$$

$$<k_6|k_{68}> = \frac{4}{9 \times 15}\int\rho^4 r^4 \qquad {}^3P_o \quad \Psi_2 \quad \Psi_9$$

$$<k_7|k_{69}> = \frac{4}{45}\int\rho^4 r^4 \qquad {}^3P_1 \quad \Psi_2 \quad \Psi_9$$

$$<k_8|k_{70}< = \frac{4}{27}\int\rho^4 r^4 \qquad {}^3P_2 \quad \Psi_2 \quad \Psi_9$$

$$<k_3|k_{78}> = \frac{1}{2}\int(\rho^4 - r^4) \qquad {}^1S_o \quad \Psi_2 \quad \Psi_{10}$$

$$<k_4|k_{79}> = -\frac{1}{2}\int(\rho^4 - r^4) \qquad {}^3S_1 \quad \Psi_2 \quad \Psi_{10}$$

$$<k_9|k_9> = \frac{1}{3}\int\rho^2 r^2 \qquad {}^1P_1 \quad \Psi_3 \quad \Psi_3$$

$$<k_{10}|k_{10}> = \frac{2}{27}\int\rho^2 r^2 \qquad {}^3P_o \quad \Psi_3 \quad \Psi_3$$

$$<k_{11}|k_{11}> = \frac{1}{18}\int\rho^2 r^2 \qquad {}^3P_1 \quad \Psi_3 \quad \Psi_3$$

$$<k_{12}|k_{12}> = \frac{1}{9}\int\rho^2 r^2 \qquad {}^3P_1 \quad \Psi_3 \quad \Psi_3$$

$$<k_{13}|k_{13}> = \frac{5}{54}\int\rho^2 r^2 \qquad {}^3P_2 \quad \Psi_3 \quad \Psi_3$$

$\langle k_{10}\|k_{16}\rangle = \frac{20}{27\sqrt{6}}\int \rho^2 r^2$	^3P_o	Ψ_3	Ψ_4
$\langle k_{11}\|k_{17}\rangle = -\frac{5}{9\sqrt{6}}\int \rho^2 r^2$	$^3P_1$	Ψ_3	Ψ_4
$\langle k_{13}\|k_{18}\rangle = -\frac{5}{27\sqrt{6}}\int \rho^2 r^2$	$^3P_2$	Ψ_3	Ψ_4
$\langle k_{10}\|k_{42}\rangle = \frac{64}{9 \times 15\sqrt{6}}\int \rho^4 r^4$	^3P_o	Ψ_3	Ψ_7
$\langle k_{11}\|k_{43}\rangle = -\frac{16}{45\sqrt{6}}\int \rho^4 r^4$	$^3P_1$	Ψ_3	Ψ_7
$\langle k_{13}\|k_{44}\rangle = -\frac{16}{9 \times 15\sqrt{6}}\int \rho^4 r^4$	$^3P_2$	Ψ_3	Ψ_7
$\langle k_{10}\|k_{68}\rangle = \frac{4}{9 \times 15}\int \rho^4 r^4$	^3P_o	Ψ_3	Ψ_9
$\langle k_{11}\|k_{69}\rangle = \frac{2}{45}\int \rho^4 r^4$	$^3P_1$	Ψ_3	Ψ_9
$\langle k_{13}\|k_{70}\rangle = -\frac{2}{27}\int \rho^4 r^4$	$^3P_2$	Ψ_3	Ψ_9
$\langle k_{14}\|k_{14}\rangle = \frac{2}{3}\int r^4$	$^3S_1$	Ψ_4	Ψ_4
$\langle k_{15}\|k_{15}\rangle = \frac{2}{3}\int \rho^4$	$^3D_1$	Ψ_4	Ψ_4
$\langle k_{16}\|k_{16}\rangle = \frac{100}{81}\int \rho^2 r^2$	^3P_o	Ψ_4	Ψ_4
$\langle k_{17}\|k_{17}\rangle = \frac{25}{27}\int \rho^2 r^2$	$^3P_1$	Ψ_4	Ψ_4
$\langle k_{18}\|k_{18}\rangle = \frac{5}{81}\int \rho^2 r^2$	$^3P_2$	Ψ_4	Ψ_4
$\langle k_{14}\|k_{35}\rangle = \frac{4}{9}\int (\rho^2 r^6 + \frac{1}{5}\rho^4 r^4)$	$^3S_1$	Ψ_4	Ψ_7

$\langle k_{15}|k_{36}\rangle = \frac{4}{9}\int(\rho^6 r^2 + \frac{1}{5}\rho^4 r^4)$ ${}^3D_1$ Ψ_4 Ψ_7

$\langle k_{16}|k_{42}\rangle = \frac{64}{81}\int\rho^4 r^4$ ${}^3P_o$ Ψ_4 Ψ_7

$\langle k_{17}|k_{43}\rangle = \frac{16}{27}\int\rho^4 r^4$ ${}^3P_1$ Ψ_4 Ψ_7

$\langle k_{18}|k_{44}\rangle = \frac{16}{5 \times 81}\int\rho^4 r^4$ ${}^3P_2$ Ψ_4 Ψ_7

$\langle k_{16}|k_{68}\rangle = \frac{8}{27\sqrt{6}}\int\rho^4 r^4$ ${}^3P_o$ Ψ_4 Ψ_9

$\langle k_{17}|k_{69}\rangle = -\frac{4}{9\sqrt{6}}\int\rho^4 r^4$ ${}^3P_1$ Ψ_4 Ψ_9

$\langle k_{18}|k_{70}\rangle = \frac{4}{27\sqrt{6}}\int\rho^4 r^4$ ${}^3P_2$ Ψ_4 Ψ_9

$\langle k_{19}|k_{19}\rangle = \frac{2}{9}\int\rho^4 r^4$ ${}^1S_o$ Ψ_5 Ψ_5

$\langle k_{20}|k_{20}\rangle = \frac{2}{45}\int\rho^4 r^4$ ${}^1D_2$ Ψ_5 Ψ_5

$\langle k_{21}|k_{21}\rangle = \frac{2}{9}\int\rho^4 r^4$ ${}^3S_1$ Ψ_5 Ψ_5

$\langle k_{22}|k_{22}\rangle = \frac{2}{9 \times 25}\int\rho^4 r^4$ ${}^3D_1$ Ψ_5 Ψ_5

$\langle k_{23}|k_{23}\rangle = \frac{2}{9 \times 15}\int\rho^4 r^4$ ${}^3D_2$ Ψ_5 Ψ_5

$\langle k_{24}|k_{24}\rangle = \frac{14}{25 \times 27}\int\rho^4 r^4$ ${}^3D_3$ Ψ_5 Ψ_5

$\langle k_{19}|k_{25}\rangle = \frac{8}{45}\int\rho^6 r^6$ ${}^1S_o$ Ψ_5 Ψ_6

$\langle k_{20}|k_{26}\rangle = \frac{16}{9 \times 35}\int\rho^6 r^6$ ${}^1D_2$ Ψ_5 Ψ_6

$\langle k_{21}|k_{28}\rangle = \frac{8}{45}\int \rho^6 r^6$ $\quad {}^3S_1 \quad \Psi_5 \quad \Psi_6$

$\langle k_{22}|k_{29}\rangle = \frac{16}{25 \text{ x } 63}\int \rho^6 r^6$ $\quad {}^3D_1 \quad \Psi_5 \quad \Psi_6$

$\langle k_{23}|k_{30}\rangle = \frac{16}{15 \text{ x } 63}\int \rho^6 r^6$ $\quad {}^3D_2 \quad \Psi_5 \quad \Psi_6$

$\langle k_{24}|k_{31}\rangle = \frac{16}{25 \text{ x } 27}\int \rho^6 r^6$ $\quad {}^3D_3 \quad \Psi_5 \quad \Psi_6$

$\langle k_{22}|k_{37}\rangle = \frac{4}{9 \text{ x } 25\sqrt{6}}\int (\rho^6 r^4 - \rho^4 r^6)$ $\quad {}^3D_1 \quad \Psi_5 \quad \Psi_7$

$\langle k_{23}|k_{38}\rangle = -\frac{4}{9 \text{ x } 15\sqrt{6}}\int (\rho^6 r^4 - \rho^4 r^6)$ $\quad {}^3D_2 \quad \Psi_5 \quad \Psi_7$

$\langle k_{24}|k_{39}\rangle = \frac{8}{25 \text{ x } 27\sqrt{6}}\int (\rho^6 r^4 - \rho^4 r^6)$ $\quad {}^3D_3 \quad \Psi_5 \quad \Psi_7$

$\langle k_{19}|k_{50}\rangle = \frac{16}{7 \text{ x } 15}\int \rho^8 r^8$ $\quad {}^1S_o \quad \Psi_5 \quad \Psi_8$

$\langle k_{20}|k_{51}\rangle = \frac{16}{9 \text{ x } 35}\int \rho^8 r^8$ $\quad {}^1D_2 \quad \Psi_5 \quad \Psi_8$

$\langle k_{21}|k_{53}\rangle = \frac{16}{7 \text{ x } 15}\int \rho^8 r^8$ $\quad {}^3S_1 \quad \Psi_5 \quad \Psi_8$

$\langle k_{22}|k_{54}\rangle = \frac{16}{25 \text{ x } 63}\int \rho^8 r^8$ $\quad {}^3D_1 \quad \Psi_5 \quad \Psi_8$

$\langle k_{23}|k_{55}\rangle = \frac{16}{15 \text{ x } 63}\int \rho^8 r^8$ $\quad {}^3D_2 \quad \Psi_5 \quad \Psi_8$

$\langle k_{24}|k_{56}\rangle = \frac{16}{25 \text{ x } 27}\int \rho^8 r^8$ $\quad {}^3D_3 \quad \Psi_5 \quad \Psi_8$

$\langle k_{19}|k_{64}\rangle = \frac{2}{9}\int (\rho^6 r^4 - \rho^4 r^6)$ $\quad {}^1S_o \quad \Psi_5 \quad \Psi_9$

$\langle k_{20}|k_{65}\rangle = \frac{2}{45}\int (\rho^6 r^4 - \rho^4 r^6)$ $\quad {}^1D_2 \quad \Psi_5 \quad \Psi_9$

$\langle k_{21}|k_{74}\rangle = -\frac{2}{9}\int (\rho^6 r^4 - \rho^4 r^6)$ $\quad {}^3S_1 \quad \Psi_5 \quad \Psi_9$

$\langle k_{22}|k_{75}\rangle = -\frac{2}{9 \times 25}\int(\rho^6 r^4 - \rho^4 r^6)$ $^3D_1$ Ψ_5 Ψ_9

$\langle k_{23}|k_{76}\rangle = -\frac{2}{9 \times 15}\int(\rho^6 r^4 - \rho^4 r^6)$ $^3D_2$ Ψ_5 Ψ_9

$\langle k_{24}|k_{77}\rangle = -\frac{14}{25 \times 27}\int(\rho^6 r^4 - \rho^4 r^6)$ $^3D_3$ Ψ_5 Ψ_9

$\langle k_{19}|k_{78}\rangle = \frac{1}{3}\int(\rho^4 r^2 + \rho^2 r^4)$ $^1S_0$ Ψ_5 Ψ_{10}

$\langle k_{21}|k_{79}\rangle = \frac{1}{3}\int(\rho^4 r^2 + \rho^2 r^4)$ $^3S_1$ Ψ_5 Ψ_{10}

$\langle k_{25}|k_{25}\rangle = \frac{32}{9 \times 25}\int\rho^8 r^8$ $^1S_0$ Ψ_6 Ψ_6

$\langle k_{26}|k_{26}\rangle = \frac{128}{45 \times 49}\int\rho^8 r^8$ $^1D_2$ Ψ_6 Ψ_6

$\langle k_{27}|k_{27}\rangle = \frac{32}{9 \times 25 \times 49}\int\rho^8 r^8$ $^1G_4$ Ψ_6 Ψ_6

$\langle k_{28}|k_{28}\rangle = \frac{32}{9 \times 25}\int\rho^8 r^8$ $^3S_1$ Ψ_6 Ψ_6

$\langle k_{29}|k_{29}\rangle = \frac{128}{9 \times 25 \times 49}\int\rho^8 r^8$ $^3D_1$ Ψ_6 Ψ_6

$\langle k_{30}|k_{30}\rangle = \frac{128}{9 \times 15 \times 49}\int\rho^8 r^8$ $^3D_2$ Ψ_6 Ψ_6

$\langle k_{31}|k_{31}\rangle = \frac{128}{7 \times 25 \times 27}\int\rho^8 r^8$ $^3D_3$ Ψ_6 Ψ_6

$\langle k_{32,J}|k_{32,J}\rangle = \frac{32}{9 \times 25 \times 49}\int\rho^8 r^8$ ^3G_J Ψ_6 Ψ_6

$\langle k_{29}|k_{37}\rangle = \frac{32}{25 \times 63\sqrt{6}}\int(\rho^8 r^6 - \rho^6 r^8)$ $^3D_1$ Ψ_6 Ψ_7

$\langle k_{30}|k_{38}\rangle = -\frac{32}{7 \times 9 \times 15\sqrt{6}}\int(\rho^8 r^6 - \rho^6 r^8)$ $^3D_2$ Ψ_6 Ψ_7

$\langle k_{31}|k_{39}\rangle = \frac{64}{9 \times 21 \times 25\sqrt{6}}\int(\rho^8 r^6 - \rho^6 r^8)$ $^3D_3$ Ψ_6 Ψ_7

$$\langle k_{25}|k_{50}\rangle = \frac{64}{21 \times 25}\int \rho^{10} r^{10} \qquad {}^1S_o \quad \Psi_6 \quad \Psi_8$$

$$\langle k_{26}|k_{51}\rangle = \frac{128}{45 \times 49}\int \rho^{10} r^{10} \qquad {}^1D_2 \quad \Psi_6 \quad \Psi_8$$

$$\langle k_{27}|k_{52}\rangle = \frac{64}{11 \times 25 \times 49}\int \rho^{10} r^{10} \qquad {}^1G_4 \quad \Psi_6 \quad \Psi_8$$

$$\langle k_{28}|k_{53}\rangle = \frac{64}{21 \times 25}\int \rho^{10} r^{10} \qquad {}^3S_1 \quad \Psi_6 \quad \Psi_8$$

$$\langle k_{29}|k_{54}\rangle = \frac{128}{9 \times 25 \times 49}\int \rho^{10} r^{10} \qquad {}^3D_1 \quad \Psi_6 \quad \Psi_8$$

$$\langle k_{30}|k_{55}\rangle = \frac{128}{9 \times 15 \times 49}\int \rho^{10} r^{10} \qquad {}^3D_2 \quad \Psi_6 \quad \Psi_8$$

$$\langle k_{31}|k_{56}\rangle = \frac{128}{9 \times 21 \times 25}\int \rho^{10} r^{10} \qquad {}^3D_3 \quad \Psi_6 \quad \Psi_8$$

$$\langle k_{32,J}|k_{57,J}\rangle = \frac{64}{11 \times 25 \times 49}\int \rho^{10} r^{10} \qquad {}^3G_J \quad \Psi_6 \quad \Psi_8$$

$$\langle k_{25}|k_{64}\rangle = \frac{8}{45}\int (\rho^8 r^6 - \rho^6 r^8) \qquad {}^1S_o \quad \Psi_6 \quad \Psi_9$$

$$\langle k_{26}|k_{65}\rangle = \frac{16}{9 \times 35}\int (\rho^8 r^6 - \rho^6 r^8) \qquad {}^1D_2 \quad \Psi_6 \quad \Psi_9$$

$$\langle k_{28}|k_{74}\rangle = -\frac{8}{45}\int (\rho^8 r^6 - \rho^6 r^8) \qquad {}^3S_1 \quad \Psi_6 \quad \Psi_9$$

$$\langle k_{29}|k_{75}\rangle = -\frac{16}{25 \times 63}\int (\rho^8 r^6 - \rho^6 r^8) \qquad {}^3D_1 \quad \Psi_6 \quad \Psi_9$$

$$\langle k_{30}|k_{76}\rangle = -\frac{16}{21 \times 45}\int (\rho^8 r^6 - \rho^6 r^8) \qquad {}^3D_2 \quad \Psi_6 \quad \Psi_9$$

$$\langle k_{31}|k_{77}\rangle = -\frac{16}{25 \times 27}\int (\rho^8 r^6 - \rho^6 r^8) \qquad {}^3D_3 \quad \Psi_6 \quad \Psi_9$$

$$\langle k_{25}|k_{78}\rangle = \frac{4}{15}\int (\rho^6 r^4 + \rho^4 r^6) \qquad {}^1S_o \quad \Psi_6 \quad \Psi_{10}$$

$$\langle k_{28}|k_{79}\rangle = \frac{4}{15}\int (\rho^6 r^4 + \rho^4 r^6) \qquad {}^3S_1 \quad \Psi_6 \quad \Psi_{10}$$

$$<k_{35}|k_{35}> = \frac{8}{27}\int(\rho^4 r^8 + \frac{2}{5}\rho^6 r^6 + \frac{1}{25}\rho^8 r^4) \qquad {}^3S_1 \quad \Psi_7 \quad \Psi_7$$

$$<k_{36}|k_{36}> = \frac{8}{27}\int(\rho^8 r^4 + \frac{2}{5}\rho^6 r^6 + \frac{1}{25}\rho^4 r^8) \qquad {}^3D_1 \quad \Psi_7 \quad \Psi_7$$

$$<k_{37}|k_{37}> = \frac{4}{25 \times 27}\int(\rho^8 r^4 - 2\rho^6 r^6 + \rho^4 r^8) \qquad {}^3D_1 \quad \Psi_7 \quad \Psi_7$$

$$<k_{38}|k_{38}> = \frac{4}{5 \times 81}\int(\rho^8 r^4 - 2\rho^6 r^6 + \rho^4 r^8) \qquad {}^3D_2 \quad \Psi_7 \quad \Psi_7$$

$$<k_{39}|k_{39}> = \frac{16}{7 \times 25 \times 81}\int(\rho^8 r^4 - 2\rho^6 r^6 + \rho^4 r^8) \qquad {}^3D_3 \quad \Psi_7 \quad \Psi_7$$

$$<k_{40}|k_{40}> = \frac{16}{21 \times 25}\int\rho^4 r^8 \qquad {}^3D_3 \quad \Psi_7 \quad \Psi_7$$

$$<k_{41}|k_{41}> = \frac{16}{21 \times 25}\int\rho^8 r^4 \qquad {}^3G_3 \quad \Psi_7 \quad \Psi_7$$

$$<k_{42}|k_{42}> = \frac{32 \times 32}{45 \times 45}\int\rho^6 r^6 \qquad {}^3P_0 \quad \Psi_7 \quad \Psi_7$$

$$<k_{43}|k_{43}> = \frac{16 \times 16}{25 \times 27}\int\rho^6 r^6 \qquad {}^3P_1 \quad \Psi_7 \quad \Psi_7$$

$$<k_{44}|k_{44}> = \frac{16 \times 16}{9 \times 15 \times 75}\int\rho^6 r^6 \qquad {}^3P_2 \quad \Psi_7 \quad \Psi_7$$

$$<k_{45}|k_{45}> = \frac{32}{15 \times 25}\int\rho^6 r^6 \qquad {}^3P_2 \quad \Psi_7 \quad \Psi_7$$

$$<k_{46}|k_{46}> = \frac{32}{15 \times 25}\int\rho^6 r^6 \qquad {}^3F_2 \quad \Psi_7 \quad \Psi_7$$

$$<k_{47}|k_{47}> = \frac{64}{5 \times 25 \times 49}\int\rho^6 r^6 \qquad {}^3F_2 \quad \Psi_7 \quad \Psi_7$$

$$<k_{48}|k_{48}> = \frac{4}{7 \times 25}\int\rho^6 r^6 \qquad {}^3F_3 \quad \Psi_7 \quad \Psi_7$$

$$<k_{49}|k_{49}> = \frac{4}{25 \times 49}\int\rho^6 r^6 \qquad {}^3F_4 \quad \Psi_7 \quad \Psi_7$$

$$<k_{37}|k_{54}> = \frac{32}{25 \times 63\sqrt{6}}\int(\rho^{10} r^8 - \rho^8 r^{10}) \qquad {}^3D_1 \quad \Psi_7 \quad \Psi_8$$

$$<k_{38}|k_{55}> = \frac{-32}{21 \times 45\sqrt{6}}\int(\rho^{10} r^8 - \rho^8 r^{10}) \qquad {}^3D_2 \quad \Psi_7 \quad \Psi_8$$

$$\langle k_{39}|k_{56}\rangle = \frac{64}{9 \text{ x } 21 \text{ x } 25\sqrt{6}} \int (\rho^{10}r^{8} - \rho^{8}r^{10}) \qquad {}^{3}D_{3} \quad \Psi_7 \quad \Psi_8$$

$$\langle k_{37}|k_{75}\rangle = -\frac{4}{9 \text{ x } 25 \text{ x}\sqrt{6}} \int (\rho^{8}r^{4} - 2\rho^{6}r^{6} + \rho^{4}r^{8}) \qquad {}^{3}D_{1} \quad \Psi_7 \quad \Psi_9$$

$$\langle k_{38}|k_{76}\rangle = \frac{4}{9 \text{ x } 15\sqrt{6}} \int (\rho^{8}r^{4} - 2\rho^{6}r^{6} + \rho^{4}r^{8}) \qquad {}^{3}D_{2} \quad \Psi_7 \quad \Psi_9$$

$$\langle k_{39}|k_{77}\rangle = -\frac{8}{25 \text{ x } 27 \text{ x}\sqrt{6}} \int (\rho^{8}r^{4} - 2\rho^{6}r^{6} + \rho^{4}r^{8}) \qquad {}^{3}D_{3} \quad \Psi_7 \quad \Psi_9$$

$$\langle k_{42}|k_{68}\rangle = \frac{128}{25 \text{ x } 27\sqrt{6}} \int \rho^{6}r^{6} \qquad {}^{3}P_{o} \quad \Psi_7 \quad \Psi_9$$

$$\langle k_{43}|k_{69}\rangle = -\frac{64}{9 \text{ x } 25\sqrt{6}} \int \rho^{6}r^{6} \qquad {}^{3}P_{1} \quad \Psi_7 \quad \Psi_9$$

$$\langle k_{44}|k_{70}\rangle = \frac{64}{25 \text{ x } 27\sqrt{6}} \int \rho^{6}r^{6} \qquad {}^{3}P_{2} \quad \Psi_7 \quad \Psi_9$$

$$\langle k_{47}|k_{71}\rangle = \frac{32}{25 \text{ x } 49\sqrt{6}} \int \rho^{6}r^{6} \qquad {}^{3}F_{2} \quad \Psi_7 \quad \Psi_9$$

$$\langle k_{48}|k_{72}\rangle = -\frac{8}{7 \text{ x } 25\sqrt{6}} \int \rho^{6}r^{6} \qquad {}^{3}F_{3} \quad \Psi_7 \quad \Psi_9$$

$$\langle k_{49}|k_{73}\rangle = \frac{24}{25 \text{ x } 49\sqrt{6}} \int \rho^{6}r^{6} \qquad {}^{3}F_{4} \quad \Psi_7 \quad \Psi_9$$

$$\langle k_{50}|k_{50}\rangle = \frac{128}{25 \text{ x } 49} \int \rho^{12}r^{12} \qquad {}^{1}S_{o} \quad \Psi_8 \quad \Psi_8$$

$$\langle k_{51}|k_{51}\rangle = \frac{128}{45 \text{ x } 49} \int \rho^{12}r^{12} \qquad {}^{1}D_{2} \quad \Psi_8 \quad \Psi_8$$

$$\langle k_{52}|k_{52}\rangle = \frac{18 \text{ x } 64}{25 \text{ x } 49 \text{ x } 121} \int \rho^{12}r^{12} \qquad {}^{1}G_{4} \quad \Psi_8 \quad \Psi_8$$

$$\langle k_{53}|k_{53}\rangle = \frac{128}{25 \text{ x } 49} \int \rho^{12}r^{12} \qquad {}^{3}S_{1} \quad \Psi_8 \quad \Psi_8$$

$$\langle k_{54}|k_{54}\rangle = \frac{128}{9 \text{ x } 25 \text{ x } 49} \int \rho^{12}r^{12} \qquad {}^{3}D_{1} \quad \Psi_8 \quad \Psi_8$$

$$\langle k_{55}|k_{55}\rangle = \frac{128}{9 \text{ x } 15 \text{ x } 49} \int \rho^{12}r^{12} \qquad {}^{3}D_{2} \quad \Psi_8 \quad \Psi_8$$

$$\langle k_{56}|k_{56}\rangle = \frac{128}{7 \text{ x } 25 \text{ x } 27} \int \rho^{12}r^{12} \qquad {}^{3}D_{3} \quad \Psi_8 \quad \Psi_8$$

$\langle k_{57,J}|k_{57,J}\rangle = \frac{18 \times 64}{25 \times 49 \times 121}\int \rho^{12}r^{12}$ ^3G_J Ψ_8 Ψ_8

$\langle k_{60}|k_{60}\rangle = \frac{128}{9 \times 13 \times 49 \times 121}\int \rho^{12}r^{12}$ $^1I_6$ Ψ_8 Ψ_8

$\langle k_{61,J}|k_{61,J}\rangle = \frac{128}{9 \times 13 \times 49 \times 121}\int \rho^{12}r^{12}$ ^3I_J Ψ_8 Ψ_8

$\langle k_{50}|k_{64}\rangle = \frac{16}{7 \times 15}\int (\rho^{10}r^{8} - \rho^{8}r^{10})$ ^1S_o Ψ_8 Ψ_9

$\langle k_{51}|k_{65}\rangle = \frac{16}{9 \times 35}\int (\rho^{10}r^{8} - \rho^{8}r^{10})$ $^1D_2$ Ψ_8 Ψ_9

$\langle k_{53}|k_{74}\rangle = - \frac{16}{7 \times 15}\int (\rho^{10}r^{8} - \rho^{8}r^{10})$ $^3S_1$ Ψ_8 Ψ_9

$\langle k_{54}|k_{75}\rangle = - \frac{16}{25 \times 63}\int (\rho^{10}r^{8} - \rho^{8}r^{10})$ $^3D_1$ Ψ_8 Ψ_9

$\langle k_{55}|k_{76}\rangle = - \frac{16}{15 \times 63}\int (\rho^{10}r^{8} - \rho^{8}r^{10})$ $^3D_2$ Ψ_8 Ψ_9

$\langle k_{56}|k_{77}\rangle = - \frac{16}{25 \times 27}\int (\rho^{10}r^{8} - \rho^{8}r^{10})$ $^3D_3$ Ψ_8 Ψ_9

$\langle k_{50}|k_{78}\rangle = \frac{8}{35}\int (\rho^{8}r^{6} + \rho^{6}r^{8})$ ^1S_o Ψ_8 Ψ_{10}

$\langle k_{53}|k_{79}\rangle = \frac{8}{35}\int (\rho^{8}r^{6} + \rho^{6}r^{8})$ $^3S_1$ Ψ_8 Ψ_{10}

$\langle k_{64}|k_{64}\rangle = \frac{2}{9}\int (\rho^{8}r^{4} - 2\rho^{6}r^{6} + \rho^{4}r^{8})$ ^1S_o Ψ_9 Ψ_9

$\langle k_{65}|k_{65}\rangle = \frac{2}{45}\int (\rho^{8}r^{4} - 2\rho^{6}r^{6} + \rho^{4}r^{8})$ $^1D_2$ Ψ_9 Ψ_9

$\langle k_{66}|k_{66}\rangle = \frac{8}{75}\int \rho^{6}r^{6}$ $^1P_1$ Ψ_9 Ψ_9

$\langle k_{67}|k_{67}\rangle = \frac{8}{7 \times 25}\int \rho^{6}r^{6}$ $^1F_3$ Ψ_9 Ψ_9

$\langle k_{68}|k_{68}\rangle = \frac{8}{25 \times 27}\int \rho^{6}r^{6}$ ^3P_o Ψ_9 Ψ_9

$$\langle k_{69}|k_{69}\rangle = \frac{8}{9 \text{ x } 25}\int \rho^6 r^6 \qquad {}^3P_1 \quad \Psi_9 \quad \Psi_9$$

$$\langle k_{70}|k_{70}\rangle = \frac{8}{9 \text{ x } 15}\int \rho^6 r^6 \qquad {}^3P_2 \quad \Psi_9 \quad \Psi_9$$

$$\langle k_{71}|k_{71}\rangle = \frac{8}{15 \text{ x } 49}\int \rho^6 r^6 \qquad {}^3F_2 \quad \Psi_9 \quad \Psi_9$$

$$\langle k_{72}|k_{72}\rangle = \frac{8}{21 \text{ x } 25}\int \rho^6 r^6 \qquad {}^3F_3 \quad \Psi_9 \quad \Psi_9$$

$$\langle k_{73}|k_{73}\rangle = \frac{24}{25 \text{ x } 49}\int \rho^6 r^6 \qquad {}^3F_4 \quad \Psi_9 \quad \Psi_9$$

$$\langle k_{74}|k_{74}\rangle = \frac{2}{9}\int (\rho^8 r^4 - 2\rho^6 r^6 + \rho^4 r^8) \qquad {}^3S_1 \quad \Psi_9 \quad \Psi_9$$

$$\langle k_{75}|k_{75}\rangle = \frac{2}{9 \text{ x } 25}\int (\rho^8 r^4 - 2\rho^6 r^6 + \rho^4 r^8) \qquad {}^3D_1 \quad \Psi_9 \quad \Psi_9$$

$$\langle k_{76}|k_{76}\rangle = \frac{2}{9 \text{ x } 15}\int (\rho^8 r^4 - 2\rho^6 r^6 + \rho^4 r^8) \qquad {}^3D_2 \quad \Psi_9 \quad \Psi_9$$

$$\langle k_{77}|k_{77}\rangle = \frac{14}{25 \text{ x } 27}\int (\rho^8 r^4 - 2\rho^6 r^6 + \rho^4 r^8) \qquad {}^3D_3 \quad \Psi_9 \quad \Psi_9$$

$$\langle k_{64}|k_{78}\rangle = \frac{1}{3}\int (\rho^6 r^2 - \rho^2 r^6) \qquad {}^1S_o \quad \Psi_9 \quad \Psi_{10}$$

$$\langle k_{74}|k_{78}\rangle = -\frac{1}{3}\int (\rho^6 r^2 - \rho^2 r^6) \qquad {}^3S_1 \quad \Psi_9 \quad \Psi_{10}$$

$$\langle k_{78}|k_{78}\rangle = \frac{1}{2}\int (\rho^4 + 2\rho^2 r^2 + r^4) \qquad {}^1S_o \quad \Psi_{10} \quad \Psi_{10}$$

$$\langle k_{79}|k_{79}\rangle = \frac{1}{2}\int (\rho^4 + 2\rho^2 r^2 + r^4) \qquad {}^3S_1 \quad \Psi_{10} \quad \Psi_{10}$$

TABLE III-3

Off-Diagonal Potential Energy Matrix Elements

The off-diagonal matrix elements arise because of the tensor operator in the potential. The tensor operator is defined $S_{12} = \frac{3}{\rho^2} T_{ij}(\rho,\rho)T_{ij}(\sigma^{(1)},\sigma^{(2)})$. The matrix elements in integral form are listed below. The same conventions as used in Table II are used.

$\langle k_2 \| S_{12} \| k_{15} \rangle = -\frac{4}{\sqrt{6}} \int \rho^2$	$^3S_1/^3D_1$	Ψ_1	Ψ_4
$\langle k_2 \| S_{12} \| k_{36} \rangle = -\frac{8}{3\sqrt{6}} \int (\rho^4 r^2 + \frac{1}{5} \rho^2 r^4)$	$^3S_1/^3D_1$	Ψ_1	Ψ_7
$\langle k_4 \| S_{12} \| k_{15} \rangle = \frac{4}{\sqrt{6}} \int (\rho^4 - \rho^2 r^2)$	$^3S_1/^3D_1$	Ψ_2	Ψ_4
$\langle k_4 \| S_{12} \| k_{36} \rangle = \frac{8}{3\sqrt{6}} \int (\rho^6 r^2 - \frac{4}{5} \rho^4 r^4 - \frac{1}{5} \rho^2 r^6)$	$^3S_1/^3D_1$	Ψ_2	Ψ_7
$\langle k_8 \| S_{12} \| k_{46} \rangle = \frac{32}{25\sqrt{6}} \int \rho^4 r^4$	$^3P_2/^3F_2$	Ψ_2	Ψ_7
$\langle k_{13} \| S_{12} \| k_{46} \rangle = -\frac{16}{25\sqrt{6}} \int \rho^4 r^4$	$^3P_2/^3F_2$	Ψ_3	Ψ_7
$\langle k_{14} \| S_{12} \| k_{22} \rangle = -\frac{8}{15\sqrt{6}} \int \rho^2 r^4$	$^3S_1/^3D_1$	Ψ_4	Ψ_5
$\langle k_{15} \| S_{12} \| k_{21} \rangle = -\frac{8}{3\sqrt{6}} \int \rho^4 r^2$	$^3S_1/^3D_1$	Ψ_4	Ψ_5

$$\langle k_{14}|S_{12}|k_{29}\rangle = -\frac{64}{105\sqrt{6}}\int \rho^4 r^6 \qquad {}^3S_1/{}^3D_1 \quad \Psi_4 \quad \Psi_6$$

$$\langle k_{15}|S_{12}|k_{28}\rangle = -\frac{32}{15\sqrt{6}}\int \rho^6 r^4 \qquad {}^3S_1/{}^3D_1 \quad \Psi_4 \quad \Psi_6$$

$$\langle k_{14}|S_{12}|k_{37}\rangle = -\frac{8}{45}\int (\rho^4 r^4 - \rho^2 r^6) \qquad {}^3S_1/{}^3D_1 \quad \Psi_4 \quad \Psi_7$$

$$\langle k_{18}|S_{12}|k_{46}\rangle = \frac{16}{75}\int \rho^4 r^4 \qquad {}^3P_2/{}^3F_2 \quad \Psi_4 \quad \Psi_7$$

$$\langle k_{14}|S_{12}|k_{54}\rangle = -\frac{64}{105\sqrt{6}}\int \rho^6 r^8 \qquad {}^3S_1/{}^3D_1 \quad \Psi_4 \quad \Psi_8$$

$$\langle k_{15}|S_{12}|k_{53}\rangle = -\frac{64}{35\sqrt{6}}\int \rho^8 r^6 \qquad {}^3S_1/{}^3D_1 \quad \Psi_4 \quad \Psi_8$$

$$\langle k_{14}|S_{12}|k_{75}\rangle = \frac{8}{15\sqrt{6}}\int (\rho^4 r^4 - \rho^2 r^6) \qquad {}^3S_1/{}^3D_1 \quad \Psi_4 \quad \Psi_9$$

$$\langle k_{15}|S_{12}|k_{74}\rangle = \frac{8}{3\sqrt{6}}\int (\rho^6 r^2 - \rho^4 r^4) \qquad {}^3S_1/{}^3D_1 \quad \Psi_4 \quad \Psi_9$$

$$\langle k_{15}|S_{12}|k_{79}\rangle = -\frac{4}{\sqrt{6}}\int (\rho^4 + \rho^2 r^2) \qquad {}^3S_1/{}^3D_1 \quad \Psi_4 \quad \Psi_{10}$$

$$\langle k_{21}|S_{12}|k_{36}\rangle = -\frac{16}{9\sqrt{6}}\int (\rho^6 r^4 + \frac{1}{5}\rho^4 r^6) \qquad {}^3S_1/{}^3D_1 \quad \Psi_5 \quad \Psi_7$$

$$\langle k_{22}|S_{12}|k_{35}\rangle = -\frac{16}{45\sqrt{6}}\int (\rho^4 r^6 + \frac{1}{5}\rho^6 r^4) \qquad {}^3S_1/{}^3D_1 \quad \Psi_5 \quad \Psi_7$$

$$\langle k_{24}|S_{12}|k_{41}\rangle = -\frac{32}{7 \times 25\sqrt{6}}\int \rho^6 r^4 \qquad {}^3D_3/{}^3G_3 \quad \Psi_5 \quad \Psi_7$$

$$\langle k_{28}|S_{12}|k_{36}\rangle = -\frac{64}{45\sqrt{6}}\int (\rho^8 r^6 + \frac{1}{5}\rho^6 r^8) \qquad {}^3S_1/{}^3D_1 \quad \Psi_6 \quad \Psi_7$$

$$\langle k_{29}|S_{12}|k_{35}\rangle = -\frac{128}{7 \times 45\sqrt{6}}\int (\rho^6 r^8 + \frac{1}{5}\rho^8 r^6) \qquad {}^3S_1/{}^3D_1 \quad \Psi_6 \quad \Psi_7$$

$$\langle k_{31}|S_{12}|k_{41}\rangle = -\frac{256}{25\times 49\sqrt{6}}\int \rho^8 r^6 \qquad {}^3D_3/{}^3G_3 \quad \Psi_6 \quad \Psi_7$$

$$\langle k_{32}|S_{12}|k_{40}\rangle = -\frac{128}{49\times 75\sqrt{6}}\int \rho^6 r^8 \qquad {}^3D_3/{}^3G_3 \quad \Psi_6 \quad \Psi_7$$

$$\begin{aligned}\langle k_{35}|S_{12}|k_{37}\rangle = -\frac{16}{135}\int (&\tfrac{1}{5}\rho^8 r^4 \\ &+ \tfrac{4}{5}\rho^6 r^6 - \rho^4 r^8) \qquad {}^3D_1/{}^3S_1 \quad \Psi_7 \quad \Psi_7\end{aligned}$$

$$\langle k_{39}|S_{12}|k_{41}\rangle = -\frac{64}{49\times 75}\int (\rho^8 r^4 - \rho^6 r^6) \qquad {}^3S_1/{}^3D_1 \quad \Psi_7 \quad \Psi_7$$

$$\langle k_{44}|S_{12}|k_{46}\rangle = \frac{256}{25\times 75}\int \rho^6 r^6 \qquad {}^3P_2/{}^3F_2 \quad \Psi_7 \quad \Psi_7$$

$$\langle k_{45}|S_{12}|k_{47}\rangle = -\frac{3\times 128}{35\times 125}\int \rho^6 r^6 \qquad {}^3P_2/{}^3F_2 \quad \Psi_7 \quad \Psi_7$$

$$\begin{aligned}\langle k_{35}|S_{12}|k_{54}\rangle = -\frac{128}{7\times 45\sqrt{6}}\int (&\rho^8 r^{10} \\ &+ \tfrac{1}{5}\rho^{10} r^8) \qquad {}^3S_1/{}^3D_1 \quad \Psi_7 \quad \Psi_8\end{aligned}$$

$$\begin{aligned}\langle k_{36}|S_{12}|k_{53}\rangle = -\frac{128}{7\times 15\sqrt{6}}\int (&\rho^{10} r^8 \\ &+ \tfrac{1}{5}\rho^8 r^{10}) \qquad {}^3S_1/{}^3D_1 \quad \Psi_7 \quad \Psi_8\end{aligned}$$

$$\langle k_{40}|S_{12}|k_{57}\rangle = -\frac{6\times 128}{11\times 25\times 49\sqrt{6}}\int \rho^8 r^{10} \qquad {}^3D_3/{}^3G_3 \quad \Psi_7 \quad \Psi_8$$

$$\langle k_{41}|S_{12}|k_{56}\rangle = -\frac{256}{25\times 49\sqrt{6}}\int \rho^{10} r^8 \qquad {}^3D_3/{}^3G_3 \quad \Psi_7 \quad \Psi_8$$

$$\begin{aligned}\langle k_{35}|S_{12}|k_{75}\rangle = \frac{16}{45\sqrt{6}}\int (&\tfrac{4}{5}\rho^6 r^6 \\ &+ \tfrac{1}{5}\rho^8 r^4 - \rho^4 r^8) \qquad {}^3S_1/{}^3D_1 \quad \Psi_7 \quad \Psi_9\end{aligned}$$

$$\langle k_{36}|S_{12}|k_{74}\rangle = \frac{16}{9\sqrt{6}} \int (\rho^8 r^4 - \frac{4}{5}\,\rho^6 r^6 - \frac{1}{5}\,\rho^4 r^8) \qquad {}^3S_1/{}^3D_1 \quad \Psi_7 \quad \Psi_9$$

$$\langle k_{41}|S_{12}|k_{77}\rangle = \frac{32}{7 \times 25\sqrt{6}} \int (\rho^8 r^4 - \rho^6 r^6) \qquad {}^3D_3/{}^3G_3 \quad \Psi_7 \quad \Psi_9$$

$$\langle k_{45}|S_{12}|k_{71}\rangle = -\frac{3 \times 64}{35 \times 25\sqrt{6}} \int \rho^6 r^6 \qquad {}^3P_2/{}^3F_2 \quad \Psi_7 \quad \Psi_9$$

$$\langle k_{46}|S_{12}|k_{70}\rangle = \frac{64}{125\sqrt{6}} \int \rho^6 r^6 \qquad {}^3P_2/{}^3F_2 \quad \Psi_7 \quad \Psi_9$$

$$\langle k_{36}|S_{12}|k_{79}\rangle = -\frac{8}{3\sqrt{6}} \int (\rho^6 r^2 + \frac{6}{5}\,\rho^4 r^4 + \frac{1}{5}\,\rho^2 r^6) \qquad {}^3S_1/{}^3D_1 \quad \Psi_7 \quad \Psi_{10}$$

TABLE III-4

This table indicates our notation for the various two-body states. The pure two-body states (good LSJ) may have a tensor part incorporated, whereas the states coupled by the tensor operator have to be multiplied by the factor obtained from $\langle LSJ|S_{12}|L+2SJ\rangle$.

State	Function of r which is the potential.
$^1S_0$	V_1
$^1D_2$	V_2
$^3P_0$	V_3
$^3P_1$	V_4
$^1P_1$	V_5
$^3D_2$	V_6
$^3S_1$	V_7
$^3D_1$	V_8
$^3S_1/^3D_1$	V_9
$^3P_2$	V_{10}
$^3D_3$	V_{11}
$^1G_4$	V_{12}
^3G_J	V_{13}
$^3G_3$	V_{14}
$^3F_2$	V_{15}
$^3F_3$	V_{16}

State	Function of r which is the potential.
$^3F_4$	V_{17}
$^3P_2/^3F_2$	V_{18}
$^3D_3/^3G_3$	V_{19}
$^1I_6$	V_{20}
^3I_J	V_{21}
$^1F_3$	V_{22}

TABLE III-5

Potential Energy Matrix Elements

$$<\Psi_1|V|\Psi_1> \;=\; \frac{1}{2}\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i+\lambda_j}\right)^3 (A_1+A_7)\,\frac{1}{\sqrt{\pi}}$$

$$<\Psi_1|V|\Psi_2> \;=\; \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i+\lambda_j}\right)^3 \frac{\lambda_j}{\lambda_i+\lambda_j}\,[B_1-B_7-\frac{3}{2}\,(A_1-A_7)]\,\frac{1}{\sqrt{\pi}}$$

$$<\Psi_1|V|\Psi_3> \;=\; o$$

$$<\Psi_1|V|\Psi_4> \;=\; -\,\frac{8}{\sqrt{6}}\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i+\lambda_j}\right)^3 \frac{\lambda_j}{\lambda_i+\lambda_j}\,B_9\,\frac{1}{\sqrt{\pi}}$$

$$<\Psi_1|V|\Psi_5> \;=\; 2\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i+\lambda_j}\right)^3 \left(\frac{\lambda_j}{\lambda_i+\lambda_j}\right)^2 (B_1+B_7)\,\frac{1}{\sqrt{\pi}}$$

$$<\Psi_1|V|\Psi_6> \;=\; \frac{\sqrt{70}}{5 \times 7 \times 9}\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i+\lambda_j}\right)^7 \frac{\lambda_j{}^2}{\lambda_i{}^2}\,(C_1+C_7)\,\frac{1}{\sqrt{\pi}}$$

$$<\Psi_1|V|\Psi_7> \;=\; -\,\frac{8}{\sqrt{385}\sqrt{6}}\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i+\lambda_j}\right)^5 \frac{\lambda_j{}^2}{\lambda_i(\lambda_i+\lambda_j)}\,(C_9+\frac{1}{2}\,B_9)\,\frac{1}{\sqrt{\pi}}$$

$$<\Psi_1|V|\Psi_8> \;=\; \frac{2}{15\sqrt{3 \times 7 \times 11 \times 13}}\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i+\lambda_j}\right)^9$$

$$\frac{\lambda_j{}^3}{\lambda_i{}^3}\,(D_1+D_7)\,\frac{1}{\sqrt{\pi}}$$

$$<\Psi_1|V|\Psi_9> \;=\; \frac{1}{\sqrt{105}}\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i+\lambda_j}\right)^5 \frac{\lambda_j{}^2}{(\lambda_i+\lambda_j)\lambda_i}$$

$$[C_1-C_7-\frac{5}{2}\,(B_1-B_7)]\,\frac{1}{\sqrt{\pi}}$$

$$<\Psi_1|V|\Psi_{10}> = \frac{\lambda_i + \lambda_j}{\lambda_i} \left(\frac{2\sqrt{\lambda_i \lambda_j}}{\lambda_i + \lambda_j} \right)^5 [\frac{1}{4} (B_1+B_7)$$

$$+ \frac{3}{8} (A_1+A_7)] \frac{1}{\sqrt{\pi}}$$

$$<\Psi_2|V|\Psi_2> = \left(\frac{2\sqrt{\lambda_i \lambda_j}}{\lambda_i + \lambda_j} \right)^5 [\frac{1}{2} (C_1+C_7) + \frac{3}{2} (-B_1 + \frac{2}{27} B_3$$

$$+ \frac{2}{9} B_4 + \frac{2}{3} B_5 - B_7 + \frac{10}{27} B_{10})$$

$$+ \frac{15}{8} (A_1+A_7)] \frac{1}{\sqrt{\pi}}$$

$$<\Psi_2|V|\Psi_3> = \frac{3}{2} \left(\frac{2\sqrt{\lambda_i \lambda_j}}{\lambda_i + \lambda_j} \right)^5 (\frac{2}{27} B_3 + \frac{1}{9} B_4 - \frac{5}{27} B_{10}) \frac{1}{\sqrt{\pi}}$$

$$<\Psi_2|V|\Psi_4> = \frac{1}{\sqrt{6}} \left(\frac{2\sqrt{\lambda_i \lambda_j}}{\lambda_i + \lambda_j} \right)^5 [\frac{3}{2} (\frac{20}{27} B_3 - \frac{10}{9} B_4 - 4B_9$$

$$+ \frac{10}{27} B_{10}) + 4C_9] \frac{1}{\sqrt{\pi}}$$

$$<\Psi_2|V|\Psi_5> = \left(\frac{2\sqrt{\lambda_i \lambda_j}}{\lambda_i + \lambda_j} \right)^5 \frac{\lambda_j}{\lambda_i + \lambda_j} [C_1-C_7- \frac{5}{2} (B_1-B_7)] \frac{1}{\sqrt{\pi}}$$

$$<\Psi_2|V|\Psi_6> = \frac{\sqrt{70}}{2 \times 7 \times 45} \left(\frac{2\sqrt{\lambda_i \lambda_j}}{\lambda_i + \lambda_j} \right)^9 \frac{\lambda_j}{\lambda_i} (1 + \frac{\lambda_j}{\lambda_i})$$

$$[D_1-D_7- \frac{7}{2} (C_1-C_7)] \frac{1}{\sqrt{\pi}}$$

$$<\Psi_2|V|\Psi_7> = \frac{1}{\sqrt{6} \times \sqrt{385}} \left(\frac{2\sqrt{\lambda_i \lambda_j}}{\lambda_i + \lambda_j} \right)^7 \frac{\lambda_j}{\lambda_i} [\frac{15}{4} (\frac{64}{135} C_3$$

$$- \frac{32}{45} C_4 - \frac{32}{15} C_9 + \frac{32}{135} C_{10} + \frac{32}{25} C_{18})$$

$$+ 4D_9 - 7B_9] \frac{1}{\sqrt{\pi}}$$

$$<\Psi_2|V|\Psi_8> = \frac{1}{15\sqrt{3 \times 7 \times 11 \times 13}} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{11} \frac{(\lambda_i + \lambda_j)}{\lambda_i}$$

$$\frac{\lambda_j^2}{\lambda_i^2} [E_1 - E_7 - \frac{9}{2} (D_1 - D_7)] \frac{1}{\sqrt{\pi}}$$

$$<\Psi_2|V|\Psi_9> = \frac{1}{\sqrt{105}} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{7} \frac{\lambda_j}{\lambda_i} [\frac{1}{2} (D_1 + D_7)$$

$$+ \frac{35}{8} (B_1 + B_7) + \frac{15}{4} (- \frac{2}{3} C_1 + \frac{4}{135} C_3$$

$$+ \frac{4}{45} C_4 + \frac{4}{15} C_5 - \frac{2}{3} C_7 + \frac{4}{27} C_{10}] \frac{1}{\sqrt{\pi}}$$

$$<\Psi_2|V|\Psi_{10}> = \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{5} [\frac{1}{2} (C_1 - C_7) - \frac{15}{8} (A_1 - A_7)] \frac{1}{\sqrt{\pi}}$$

$$<\Psi_3|V|\Psi_3> = \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{5} (\frac{1}{9} B_3 + \frac{1}{4} B_4 + \frac{1}{2} B_5 + \frac{5}{36} B_{10}) \frac{1}{\sqrt{\pi}}$$

$$<\Psi_3|V|\Psi_4> = \frac{1}{\sqrt{6}} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{5} (\frac{10}{9} B_3 - \frac{5}{6} B_4 - \frac{5}{18} B_{10}) \frac{1}{\sqrt{\pi}}$$

$$<\Psi_3|V|\Psi_5> = o$$

$$<\Psi_3|V|\Psi_6> = o$$

$$<\Psi_3|V|\Psi_7> = \frac{1}{\sqrt{6} \times \sqrt{385}} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{7} \frac{\lambda_j}{\lambda_i} (\frac{16}{9} C_3 - \frac{4}{3} C_4$$

$$- \frac{4}{9} C_{10} - \frac{12}{5} C_{18}) \frac{1}{\sqrt{\pi}}$$

$$\langle\Psi_3|V|\Psi_8\rangle = o$$

$$\langle\Psi_3|V|\Psi_9\rangle = \frac{1}{\sqrt{105}} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^7 \frac{\lambda_j}{\lambda_i} \left(\frac{1}{9} C_3 + \frac{1}{6} C_4 - \frac{5}{18} C_{10}\right) \frac{1}{\sqrt{\pi}}$$

$$\langle\Psi_3|V|\Psi_{10}\rangle = o$$

$$\langle\Psi_4|V|\Psi_4\rangle = \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^5 \left[\frac{50}{25} B_3 + \frac{25}{18} B_4 + \frac{5}{54} B_{10} + \frac{5}{2} A_7 + \frac{2}{3} C_8\right] \frac{1}{\sqrt{\pi}}$$

$$\langle\Psi_4|V|\Psi_5\rangle = \frac{1}{\sqrt{6}} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^7 \frac{\lambda_i + \lambda_j}{\lambda_i} (-B_9 - 2C_9) \frac{1}{\sqrt{\pi}}$$

$$\langle\Psi_4|V|\Psi_6\rangle = \frac{1}{\sqrt{6}} \frac{4\sqrt{70}}{5 \times 7 \times 9} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^9 \frac{\lambda_j(\lambda_i + \lambda_j)}{\lambda_i^2} (-C_9 - D_9) \frac{1}{\sqrt{\pi}}$$

$$\langle\Psi_4|V|\Psi_7\rangle = \frac{1}{\sqrt{385}} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^7 \frac{\lambda_j}{\lambda_i} \left[\frac{15}{4} \left(\frac{64}{81} C_3 + \frac{16}{27} C_4 + \frac{4}{45} C_7 + \frac{4}{45} C_8 - \frac{8}{45} C_9 + \frac{16}{405} C_{10} + \frac{16}{75} C_{18}\right) + \frac{2}{3} D_8 + \frac{105}{8} \left(\frac{4}{9} B_7 + \frac{8}{45} B_9\right)\right] \frac{1}{\sqrt{\pi}}$$

$$\langle\Psi_4|V|\Psi_8\rangle = \frac{1}{\sqrt{6}} \frac{1}{15\sqrt{3 \times 7 \times 11 \times 13}} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{11} \frac{\lambda_j^2(\lambda_i + \lambda_j)}{\lambda_i^3} (-12D_9 - 8E_9) \frac{1}{\sqrt{\pi}}$$

$$\begin{aligned} \langle \Psi_4 | V | \Psi_9 \rangle = {} & \frac{1}{\sqrt{6}} \frac{1}{\sqrt{105}} \left(\frac{2\sqrt{\lambda_i \lambda_j}}{\lambda_i + \lambda_j} \right)^7 \frac{\lambda_j}{\lambda_i} \, [\, \frac{15}{4} \, (\, \frac{8}{27} C_3 - \frac{4}{9} C_4 \\ & - \frac{32}{15} C_9 + \frac{4}{27} C_{10}) - 7B_9 + 4D_9] \, \frac{1}{\sqrt{\pi}} \end{aligned}$$

$$\langle \Psi_4 | V | \Psi_{10} \rangle = - \frac{1}{\sqrt{6}} \left(\frac{2\sqrt{\lambda_i \lambda_j}}{\lambda_i + \lambda_j} \right)^5 (4C_9 + 6B_9) \, \frac{1}{\sqrt{\pi}}$$

$$\begin{aligned} \langle \Psi_5 | V | \Psi_5 \rangle = {} & \frac{15}{4} \left(\frac{2\sqrt{\lambda_i \lambda_j}}{\lambda_i + \lambda_j} \right)^7 [\, \frac{2}{9} C_1 + \frac{2}{45} C_2 + \frac{2}{135} C_6 \\ & + \frac{2}{9} C_7 + \frac{2}{225} C_8 + \frac{14}{675} C_{11}] \, \frac{1}{\sqrt{\pi}} \end{aligned}$$

$$\begin{aligned} \langle \Psi_5 | V | \Psi_6 \rangle = {} & \frac{\sqrt{70}}{24} \left(\frac{2\sqrt{\lambda_i \lambda_j}}{\lambda_i + \lambda_j} \right)^9 \frac{\lambda_j}{\lambda_i} \, [\, \frac{8}{45} D_1 + \frac{16}{315} D_2 + \frac{16}{945} D_6 \\ & + \frac{8}{45} D_7 + \frac{16}{1575} D_8 + \frac{16}{675} D_{11}] \, \frac{1}{\sqrt{\pi}} \end{aligned}$$

$$\begin{aligned} \langle \Psi_5 | V | \Psi_7 \rangle = {} & \frac{1}{2\sqrt{385}} \, \frac{1}{\sqrt{6}} \left(\frac{2\sqrt{\lambda_i \lambda_j}}{\lambda_i + \lambda_j} \right)^9 \frac{\lambda_i + \lambda_j}{\lambda_i} \, [\, \frac{15}{4} \, (- \frac{4}{135} D_6 \\ & + \frac{4}{225} D_8 - \frac{416}{225} D_9 + \frac{8}{675} D_{11} - \frac{32}{175} D_{19}) \\ & + \frac{105}{8} \, (\, \frac{4}{135} C_6 - \frac{4}{225} C_8 - \frac{32}{45} C_9 \\ & - \frac{8}{675} C_{11})] \, \frac{1}{\sqrt{\pi}} \end{aligned}$$

$$\langle \Psi_5 | V | \Psi_8 \rangle = \frac{21}{8\sqrt{3 \times 7 \times 11 \times 13}} \left(\frac{2\sqrt{\lambda_i \lambda_j}}{\lambda_i + \lambda_j} \right)^{11} \frac{{\lambda_j}^2}{{\lambda_i}^2}$$

$$(\frac{16}{105} E_1 + \frac{16}{315} E_2 + \frac{16}{945} E_6 + \frac{16}{105} E_7$$

$$+ \frac{16}{1575} E_8 + \frac{16}{675} E_{11}) \frac{1}{\sqrt{\pi}}$$

$$<\Psi_5|V|\Psi_9> = \frac{2}{\sqrt{105}} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^7 \frac{\lambda_j}{\lambda_i + \lambda_j} [\frac{15}{4} (\frac{2}{9} D_1$$

$$+ \frac{2}{45} D_2 - \frac{2}{135} D_6 - \frac{2}{9} D_7 - \frac{2}{225} D_8$$

$$- \frac{14}{675} D_{11}) + \frac{105}{8} (- \frac{2}{9} C_1 - \frac{2}{45} C_2 + \frac{2}{135} C_6$$

$$+ \frac{2}{9} C_7 + \frac{2}{225} C_8 + \frac{14}{675} C_{11})] \frac{1}{\sqrt{\pi}}$$

$$<\Psi_5|V|\Psi_{10}> = \frac{\lambda_i}{\lambda_i + \lambda_j} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^5 [C_1+C_7+ \frac{5}{2} (B_1+B_7)] \frac{1}{\sqrt{\pi}}$$

$$<\Psi_6|V|\Psi_6> = \frac{1}{24} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{11} (\frac{32}{225} E_1 + \frac{128}{2205} E_2 + \frac{128}{135x49} E_6$$

$$+ \frac{32}{225} E_7 + \frac{128}{225x49} E_8 + \frac{128}{7x25x27} E_{11}$$

$$+ \frac{32}{9x25x49} E_{12} + \frac{32}{9x25x49} E_{13}) \frac{1}{\sqrt{\pi}}$$

$$<\Psi_6|V|\Psi_7> = \sqrt{\frac{2}{11}} \frac{1}{5 x 7 x 9} \frac{2}{\sqrt{6}} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^9 \frac{\lambda_i}{\lambda_i + \lambda_j}$$

$$[\frac{105}{8} (- \frac{32}{945} E_6 + \frac{32}{25x63} E_8 - \frac{37x64}{1575} E_9$$

$$+ \frac{64}{21x225} E_{11} - \frac{256}{1225} E_{19}) + \frac{945}{16}$$

$$\left(\frac{32}{945} D_6 - \frac{32}{25\text{x}63} D_8 - \frac{17\text{x}64}{1575} D_9 \right.$$

$$\left. - \frac{64}{21\text{x}225} D_{11} - \frac{128}{75\text{x}49} D_{19} \right) \Big] \frac{1}{\sqrt{\pi}}$$

$$<\Psi_6|V|\Psi_8> \;=\; \frac{\sqrt{110}}{240\sqrt{39}} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j} \right)^{13} \frac{\lambda_j}{\lambda_i} \left(\frac{64}{525} F_1 + \frac{128}{49\text{x}45} F_2 \right.$$

$$+ \frac{128}{9\text{x}15\text{x}49} F_6 + \frac{64}{525} F_7 + \frac{128}{9\text{x}25\text{x}49} F_8$$

$$\left. + \frac{128}{21\text{x}225} F_{11} + \frac{64}{25\text{x}49\text{x}11} [F_{12}+F_{13}] \right) \frac{1}{\sqrt{\pi}}$$

$$<\Psi_6|V|\Psi_9> \;=\; \frac{4}{5 \text{ x } 7 \text{ x } 9\sqrt{6}} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j} \right)^{9} \frac{\lambda_i}{\lambda_i + \lambda_j} \Big[\frac{105}{8} \Big(\frac{8}{45} E_1$$

$$+ \frac{16}{315} E_2 - \frac{16}{21\text{x}45} E_6 - \frac{8}{45} E_7 - \frac{16}{25\text{x}63} E_8$$

$$- \frac{16}{675} E_{11} \Big) + \frac{945}{16} \Big(- \frac{8}{45} D_1 - \frac{16}{315} D_2$$

$$+ \frac{16}{21\text{x}45} D_6 + \frac{8}{45} D_7 + \frac{16}{25\text{x}63} D_8$$

$$+ \frac{16}{675} D_{11} \Big) \Big] \frac{1}{\sqrt{\pi}}$$

$$<\Psi_6|V|\Psi_{10}> \;=\; \frac{\sqrt{70}}{5 \text{ x } 7 \text{ x } 9} \; \frac{\lambda_i^{\,2}}{\lambda_j(\lambda_i + \lambda_j)} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j} \right)^{7}$$

$$[2(D_1+D_7) + 7\,(C_1+C_7)] \frac{1}{\sqrt{\pi}}$$

$$\langle\Psi_7|V|\Psi_7\rangle = \frac{1}{385}\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^9 \left[\ \frac{15}{4}\left(\ \frac{4}{405}E_6 + \frac{8}{675}E_7\right.\right.$$

$$+ \frac{68}{225}E_8 - \frac{16}{675}E_9 + \frac{16}{14175}E_{11} + \frac{16}{525}E_{14}$$

$$\left.- \frac{64}{3675}E_{19}\right) + \frac{105}{8}\left(\ \frac{32\times 32}{45\times 45}D_3 + \frac{256}{675}D_4\right.$$

$$- \frac{8}{405}D_6 + \frac{16}{135}D_7 + \frac{8}{75}D_8 - \frac{64}{675}D_9$$

$$+ \frac{224}{75\times 27}D_{10} - \frac{32}{14175}D_{11} + \frac{11\times 32}{49\times 75}D_{15}$$

$$+ \frac{4}{175}D_{16} + \frac{4}{1225}D_{17} + \frac{128}{21\times 125}D_{18}$$

$$\left.+ \frac{64}{3675}D_{19}\right) + \frac{945}{16}\left(\ \frac{4}{405}C_6 + \frac{8}{27}C_7\right.$$

$$\left.\left.+ \frac{4}{225}C_8 + \frac{16}{135}C_9 + \frac{64}{2025}C_{11}\right)\right]\ \frac{1}{\sqrt{\pi}}$$

$$\langle\Psi_7|V|\Psi_8\rangle = \frac{1}{45\sqrt{385}\ \sqrt{3\times 7\times 11\times 13}}\ \frac{1}{\sqrt{6}}\left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{13}$$

$$\frac{\lambda_j(\lambda_i + \lambda_j)}{\lambda_i^{\,2}}\left[\ \frac{945}{16}\left(- \frac{32}{21\times 45}F_6\right.\right.$$

$$+ \frac{32}{25\times 63}F_8 - \frac{16\times 128}{1575}F_9 + \frac{64}{21\times 225}F_{11}$$

$$\left.- \frac{256}{25\times 49}F_{19}\right) + \frac{11\times 9\times 7\times 5\times 3}{32}\left(\ \frac{32}{21\times 45}E_6\right.$$

$$- \frac{32}{25\times 63}E_8 - \frac{8\times 128}{1575}E_9 - \frac{64}{21\times 225}E_{11}$$

$$- \frac{768}{11\mathrm{x}25\mathrm{x}49} E_{19})] \frac{1}{\sqrt{\pi}}$$

$$<\Psi_7|V|\Psi_9> = \frac{1}{35\sqrt{33}\ \sqrt{6}} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^9 [\frac{15}{4} (\frac{4}{135} E_6 - \frac{4}{225} E_8$$

$$+ \frac{416}{225} E_9 - \frac{8}{675} E_{11} + \frac{32}{175} E_{19})$$

$$+ \frac{105}{8} (\frac{128}{675} D_3 - \frac{64}{225} D_4 - \frac{8}{135} D_6$$

$$+ \frac{8}{225} D_8 - \frac{256}{225} D_9 + \frac{64}{675} D_{10} + \frac{16}{675} D_{11}$$

$$+ \frac{32}{25\mathrm{x}49} D_{15} - \frac{8}{175} D_{16} + \frac{24}{25\mathrm{x}49} D_{17}$$

$$+ \frac{256}{875} D_{18} - \frac{32}{175} D_{19}) + \frac{945}{16} (\frac{4}{135} C_6$$

$$- \frac{4}{225} C_8 - \frac{32}{45} C_9 - \frac{8}{675} C_{11})] \frac{1}{\sqrt{\pi}}$$

$$<\Psi_7|V|\Psi_{10}> = - \frac{8}{3\sqrt{6}\ \mathrm{x}\ \sqrt{385}} \frac{\lambda_i}{\lambda_j} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^7 (\frac{3}{2} D_9 + \frac{9}{2} C_9$$

$$+ \frac{21}{8} B_9) \frac{1}{\sqrt{\pi}}$$

$$<\Psi_8|V|\Psi_8> = \frac{4}{45\ \mathrm{x}\ 64} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{15} (\frac{128}{25\mathrm{x}49} G_1 + \frac{128}{45\mathrm{x}49} G_2$$

$$+ \frac{128}{9\mathrm{x}15\mathrm{x}49} G_6 + \frac{128}{25\mathrm{x}49} G_7 + \frac{128}{9\mathrm{x}25\mathrm{x}49} G_8$$

$$+ \frac{128}{7\mathrm{x}25\mathrm{x}27} G_{11} + \frac{18\mathrm{x}64}{25\mathrm{x}49\mathrm{x}121} G_{12}$$

$$+ \frac{18\times 64}{25\times 49\times 121} G_{13} + \frac{128}{9\times 49\times 121\times 13} G_{20}$$

$$+ \frac{128}{9\times 49\times 121\times 13} G_{21}) \frac{1}{\sqrt{\pi}}$$

$$\langle\Psi_8|V|\Psi_9\rangle = \frac{4}{45 \times 3 \times 7\sqrt{5 \times 11 \times 13}} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{11} \frac{\lambda_i^{\;2}}{\lambda_j(\lambda_i + \lambda_j)}$$

$$[\ \frac{945}{16} (\ \frac{16}{105} F_1 + \frac{16}{315} F_2 - \frac{16}{15\times 63} F_6$$

$$- \frac{16}{105} F_7 - \frac{16}{25\times 63} F_8 - \frac{16}{27\times 25} F_{11})$$

$$+ \frac{11!!}{32} (- \frac{16}{105} E_1 - \frac{16}{315} E_2 + \frac{16}{15\times 63} E_6$$

$$+ \frac{16}{105} E_7 + \frac{16}{25\times 63} E_8 + \frac{16}{27\times 25} E_{11})]\ \frac{1}{\sqrt{\pi}}$$

$$\langle\Psi_8|V|\Psi_{10}\rangle = \frac{1}{45\sqrt{3 \times 7 \times 11 \times 13}} \times \frac{\lambda_i^{\;2}(\lambda_i + \lambda_j)}{\lambda_j^{\;3}} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{11}$$

$$[3(E_1+E_7) + \frac{27}{2} (D_1+D_7)]\ \frac{1}{\sqrt{\pi}}$$

$$\langle\Psi_9|V|\Psi_9\rangle = \frac{1}{105} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^{9} [\ \frac{15}{4} (\ \frac{2}{9} E_1 + \frac{2}{45} E_2 + \frac{2}{135} E_6$$

$$+ \frac{2}{9} E_7 + \frac{2}{225} E_8 + \frac{14}{675} E_{11}) + \frac{105}{8}$$

$$(- \frac{4}{9} D_1 - \frac{4}{45} D_2 + \frac{8}{675} D_3 + \frac{8}{225} D_4$$

$$+ \frac{8}{75} D_5 - \frac{4}{135} D_6 - \frac{4}{9} D_7 - \frac{4}{225} D_8 + \frac{8}{135} D_{10}$$

$$- \frac{28}{675} D_{11} + \frac{8}{15x49} D_{15} + \frac{8}{525} D_{16}$$

$$+ \frac{24}{25x49} D_{17} + \frac{8}{175} D_{22}) + \frac{945}{16} (\frac{2}{9} C_1$$

$$+ \frac{2}{45} C_2 + \frac{2}{135} C_6 + \frac{2}{9} C_7 + \frac{2}{225} C_8$$

$$+ \frac{14}{675} C_{11})] \frac{1}{\sqrt{\pi}}$$

$$<\Psi_9|V|\Psi_{10}> = \frac{1}{\sqrt{105}} \frac{\lambda_i}{\lambda_j} \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^7 [\frac{1}{2} (D_1-D_7)$$

$$- \frac{35}{8} (B_1-B_7)] \frac{1}{\sqrt{\pi}}$$

$$<\Psi_{10}|V|\Psi_{10}> = \left(\frac{2\sqrt{\lambda_i\lambda_j}}{\lambda_i + \lambda_j}\right)^5 [\frac{1}{2} (C_1+C_7) + \frac{3}{2} (B_1+B_7)$$

$$+ \frac{15}{8} (A_1 + A_7)] \frac{1}{\sqrt{\pi}}$$

and $<\Psi_i|V|\Psi_j> = <\Psi_j|V|\Psi_i>$ for $i=1,...,10$

$j=1,...,10$

TABLE III-6

Mean-Square Radius Matrix Elements

$$<\Psi_1|R^2|\Psi_1> = \frac{1}{\lambda_i + \lambda_j} <\Psi_1|\Psi_1>$$

$$<\Psi_1|R^2|\Psi_5> = \frac{5}{3} \frac{1}{\lambda_i + \lambda_j} <\Psi_1|\Psi_5>$$

$$<\Psi_1|R^2|\Psi_6> = \frac{7}{3} \frac{1}{\lambda_i + \lambda_j} <\Psi_1|\Psi_6>$$

$$<\Psi_1|R^2|\Psi_8> = 3 \frac{1}{\lambda_i + \lambda_j} <\Psi_1|\Psi_8>$$

$$<\Psi_1|R^2|\Psi_{10}> = \frac{4}{3} \frac{1}{\lambda_i + \lambda_j} <\Psi_1|\Psi_{10}>$$

$$<\Psi_2|R^2|\Psi_2> = \frac{5}{3} \frac{1}{\lambda_i + \lambda_j} <\Psi_2|\Psi_2>$$

$$<\Psi_2|R^2|\Psi_9> = \frac{7}{3} \frac{1}{\lambda_i + \lambda_j} <\Psi_2|\Psi_9>$$

$$<\Psi_3|R^2|\Psi_3> = \frac{5}{3} \frac{1}{\lambda_i + \lambda_j} <\Psi_3|\Psi_3>$$

$$<\Psi_4|R^2|\Psi_4> = \frac{5}{3} \frac{1}{\lambda_i + \lambda_j} <\Psi_4|\Psi_4>$$

$$<\Psi_4|R^2|\Psi_7> = \frac{7}{3} \frac{1}{\lambda_i + \lambda_j} <\Psi_4|\Psi_7>$$

$$<\Psi_5|R^2|\Psi_5> = \frac{7}{3} \frac{1}{\lambda_i + \lambda_j} <\Psi_5|\Psi_5>$$

$$<\Psi_5|R^2|\Psi_6> = 3 \frac{1}{\lambda_i + \lambda_j} <\Psi_5|\Psi_6>$$

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$$\langle\Psi_5|R^2|\Psi_8\rangle = \frac{11}{3}\,\frac{1}{\lambda_i + \lambda_j}\,\langle\Psi_5|\Psi_8\rangle$$

$$\langle\Psi_5|R^2|\Psi_{10}\rangle = 2\,\frac{1}{\lambda_i + \lambda_j}\,\langle\Psi_5|\Psi_{10}\rangle$$

$$\langle\Psi_6|R^2|\Psi_6\rangle = \frac{11}{3}\,\frac{1}{\lambda_i + \lambda_j}\,\langle\Psi_6|\Psi_6\rangle$$

$$\langle\Psi_6|R^2|\Psi_8\rangle = \frac{13}{3}\,\frac{1}{\lambda_i + \lambda_j}\,\langle\Psi_6|\Psi_8\rangle$$

$$\langle\Psi_6|R^2|\Psi_{10}\rangle = \frac{8}{3}\,\frac{1}{\lambda_i + \lambda_j}\,\langle\Psi_6|\Psi_{10}\rangle$$

$$\langle\Psi_7|R^2|\Psi_7\rangle = 3\,\frac{1}{\lambda_i + \lambda_j}\,\langle\Psi_7|\Psi_7\rangle$$

$$\langle\Psi_8|R^2|\Psi_8\rangle = 5\,\frac{1}{\lambda_i + \lambda_j}\,\langle\Psi_8|\Psi_8\rangle$$

$$\langle\Psi_8|R^2|\Psi_{10}\rangle = \frac{10}{3}\,\frac{1}{\lambda_i + \lambda_j}\,\langle\Psi_8|\Psi_{10}\rangle$$

$$\langle\Psi_9|R^2|\Psi_9\rangle = 3\,\frac{1}{\lambda_i + \lambda_j}\,\langle\Psi_9|\Psi_9\rangle$$

$$\langle\Psi_{10}|R^2|\Psi_{10}\rangle = \frac{5}{3}\,\frac{1}{\lambda_i + \lambda_j}\,\langle\Psi_{10}|\Psi_{10}\rangle$$

$$\langle\Psi_s|R^2|\Psi_t\rangle = \langle\Psi_t|R^2|\Psi_s\rangle$$

The matrix elements not defined in the above list and their hermitian conjugates are zero.

CHAPTER IV

BINDING ENERGY AND MINIMIZATION PROCEDURES

In Chapter III we obtained the matrix elements of the normalization, the kinetic energy operator, and the potential energy operator. The rows and columns of the matrices were labelled by the non-linear parameters, λ_i. In this chapter we describe methods for minimizing the energy with respect to the linear parameters, a_i's, and the non-linear parameters. We also minimize a quantity called the force factor, and a quantity that increases the overall attraction of the potential.

The Rayleigh-Ritz Variational Procedure

The Rayleigh-Ritz formula gives an upper bound, E, of the ground state energy, E_o, by the following relationship.

$$E_o \leqslant E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

where Ψ is the trial function depending on the parameters a_i and λ_i. If we fix the λ_i's, we can minimize E with respect to the a_i's as follows. In the notation of Chapter III

$$\Psi = \sum_i a_i \phi_i$$

Thus $$E = \frac{\sum\limits_{i,j} a_i a_j \langle\phi_i|H|\phi_j\rangle}{\sum\limits_{i,j} a_i a_j \langle\phi_i|\phi_j\rangle} \tag{1}$$

Let $\langle\phi_i|H|\phi_j\rangle = H_{ij}$ and $\langle\phi_i|\phi_j\rangle = N_{ij}$.

Both H_{ij} and N_{ij} are symmetric under the exchange of subscripts i and j and both are independent of the a_i's. We can rewrite equation (1) in the form

$$\sum_{i,j} a_i a_j (H_{ij} - N_{ij}E) = o \tag{2}$$

Variation with respect to parameters a_k gives conditions $\frac{\partial E}{\partial a_k} = o$ for relative extrema of E. Differentiating equation (2) with respect to a_k we get the n equations

$$\sum_i (H_{ki} - EN_{ki})\, a_i = o \quad , \quad k=1,\ldots,n$$

In vector notation these equations become

$$(H - EN)\, \vec{A} = o$$

where $\vec{A}$ is an n component vector and H and N are n x n matrices. If we multiply through by N^{-1}, then

$$(N^{-1}\, H-E)\, \vec{A} = o \tag{3}$$

The condition for an extremum of E has become the solution to the matrix eigenvalue equation (3). The procedure, therefore, is to diagonalize the matrix $N^{-1}H$ and find its lowest eigenvalue with corresponding eigenvector $\vec{A}_{min}$. The components of $\vec{A}_{min}$ are the linear coefficients which give lowest energy for a given set of λ_i's. Although N and H are both symmetric matrices, $N^{-1}H$ is not necessarily symmetric. Since it is more efficient to diagonalize a symmetric matrix, we can form the symmetric matrix $\hat{H} = N^{-1/2}HN^{-1/2}$ instead. Equation (3) is equivalent to

$$(\hat{H} - E)\vec{B} = o \tag{3a}$$

where $\vec{A} = N^{-1/2}\vec{B}$. The matrix $N^{1/2}$ is defined so that $N^{1/2}N^{1/2} = N$. $N^{1/2}$ is found by transforming N into its equivalent diagonal matrix by a similarity transformation, taking the square root of each diagonal matrix element, and then using the same similarity transformation to transform back to the original basis.

Having found the a_i's corresponding to minimum energy for a particular set of λ_i's, we can calculate the potential and kinetic energy. Let us define $T_{ij} \equiv \langle\phi_i|T|\phi_j\rangle$ and $V_{ij} \equiv \langle\phi_i|V|\phi_j\rangle$. The total kinetic and total potential energy respectively are

$$\text{K.E.} = \frac{\sum\limits_{i,j} a_i a_j T_{ij}}{\sum\limits_{i,j} a_i a_j N_{ij}}$$

$$\text{P.E.} = \frac{\sum\limits_{i,j} a_i a_j V_{ij}}{\sum\limits_{i,j} a_i a_j N_{ij}}$$

For the non-linear parameters the minimization is done using a method developed by Powell (P67a). Manning (M67) has written a Fortran computer code for this procedure which we used. This method initially minimizes the energy with respect to one parameter at a time, that is, along the coordinate directions in parameter space. But after each pass of minimization along the n directions, a new direction is introduced in such a way that after n iterations the directions would have become mutually conjugate if a quadratic were minimized. As a consequence the exact minimum of a quadratic is found in n passes. This procedure is very efficient and even for a non-quadratic it usually requires fewer than n passes to find a reasonable value for the minimum. In our problem we do a minimization of the linear parameters for each set of λ_i's used in the non-linear parameter minimization procedure.

Calculation of the Force Factor

When one does a variational calculation on the triton to find the minimum energy, there are two other physical minima to which the minimization may converge. They are the configurations of three free particles when the energy is zero, and the configuration of two particles bound to each other and the third particle unbound, i.e. the deuteron state with energy -2.226MeV. These two relative minima have greater energy than the triton whose ground state energy is -8.482MeV. To avoid minimizing to either of these two relative minima, one can introduce a quantity that increases the strength of the potential in such a way as to give the experimental ground state energy. Essentially, this means that instead of solving the Schrödinger equation

$(T + V)\Psi = E\Psi$ for the eigenvalue E, we solve the equation $(T + \gamma V)\Psi = E_{exp}\,\Psi$ for γ. The factor γ is called the force factor. The philosophy behind this procedure is that the potential energy is negative so that multiplying it by a factor greater than one increases the magnitude of the potential energy and hence the binding. This factor is minimized with respect to the parameters at our disposal. When the parameters that give a minimum for γ have been found, we put $\gamma=1$ and with these parameters we calculate the binding energy. This is similar to what Delves and Blatt have done in their calculation (DB67; BD58). A further minimization of the energy may be attempted if one feels that it will increase the accuracy of the results. However, when we set $\gamma=1$, the energy must be less than the deuteron energy. Otherwise, one still has the possibility of minimizing to the deuteron ground state energy.

To calculate γ we use a self-consistent procedure. With some arbitrarily chosen initial $\gamma^{(o)}$ we calculate $E^{(o)}$ using the relationship

$$E^{(k)} = \frac{\sum\limits_{i,j} a_i^{(k)} a_j^{(k)} \left(T_{ij} + \gamma^{(k)} V_{ij}\right)}{\sum\limits_{i,j} a_i^{(k)} a_j^{(k)} N_{ij}} \qquad k=o,1,\ldots \qquad (4)$$

where $E^{(o)}$ is found by the minimization of linear parameters using the matrix method. This yields the set of coefficients $a_i^{(o)}$. Using these we find the next approximation to γ by the formula

$$\gamma^{(k+1)} = \frac{\sum_{i,j} a_i^{(k)} a_j^{(k)} (E_{exp} N_{ij} - T_{ij})}{\sum_{i,j} a_i^{(k)} a_j^{(k)} V_{ij}} \quad k=o,1,2,\ldots \qquad (5)$$

The $\gamma^{(1)}$ so obtained is used in equation (4) to calculate $E^{(1)}$ and $a_i^{(1)}$'s. This procedure is repeated until $\gamma^{(k)}$ and $\gamma^{(k+1)}$ and/or $E^{(k)}$ and E_{exp} differ by less than a preset amount. Convergence in this procedure is very fast; three or four iterations will produce changes in only the second or third decimal place of γ. There is equally fast convergence of E.

Calculation of ε and δ

Even if one employs the force factor technique outlined above, one may still not obtain an energy lower than the deuteron energy for a force factor equal to one. If this is the case, one may try to find an approximate wave function by using the same trial function but a somewhat distorted potential. The potential is modified to retain its overall features of repulsion and attraction but the strength of the repulsive part is decreased, and the strength of the attractive part is increased in order to give a net result of greater negative potential energy. We realize this situation by multiplying the repulsion by $(1-\varepsilon)$ and the attraction by $(1+\delta)$. If we denote the repulsive part of the potential by $V^{(r)}$ and the attractive part by $V^{(a)}$, we can do the same kind of self-consistent calculation for ε as we did for γ provided we fix the ratio $\frac{\delta}{\varepsilon} \equiv f$. The input ε is $\varepsilon^{(o)}$, from which $E^{(o)}$ can be calculated using

$$E^{(k)} = \frac{\sum_{i,j} a_i^{(k)} a_j^{(k)} [T_{ij} + (1-\varepsilon^{(k)}) V_{ij}^{(r)} + (1+f\varepsilon^{(k)} V_{ij}^{(a)}]}{\sum_{i,j} a_i^{(k)} a_j^{(k)} N_{ij}} \tag{5}$$

We obtain $\varepsilon^{(1)}$ using relationship

$$\varepsilon^{(k+1)} = \frac{\sum_{i,j} a_i^{(k)} a_j^{(k)} [E_{exp} N_{ij} - T_{ij} - V_{ij}]}{\sum_{i,j} a_i^{(k)} a_j^{(k)} [f\, V_{ij}^{(a)} - V_{ij}^{(r)}]} \tag{6}$$

The convergence of this process, like that of γ, is very rapid. We can minimize ε with respect to the non-linear parameters. We can then use the parameters obtained in a calculation with ε=o and determine the binding energy; or else we can use the result obtained with the distorted potential and calculate the correction to it by the use of first order perturbation theory. The energy correction is given by

$$\langle\Psi|(\varepsilon V^{(r)} - f\varepsilon V^{(a)})|\Psi\rangle. \tag{7}$$

CHAPTER V

THE POTENTIALS

The calculations were done with several potentials. The Bressel and Reid potentials are of physical interest since they have recently been developed and fit quite a number of data. These potentials have not been tested in the triton but seem to give good results in nuclear matter. The calculation with the Pease-Feshbach potential is not so much of physical interest but more as a check on the method that we employ. Calculations of the triton have been performed with this potential (PF52; BDL62) and we can compare our results with those obtained using different trial functions. To get an idea of the suitability of our trial functions with soft-core potentials, we do also a calculation with a central soft-core potential derived by Coester and Yen (CY63). The binding energy of the triton is calculated for the Coester-Yen potential with both exponential and Gaussian type trial functions that we use throughout the rest of our work.

The Reid Potential

The Reid soft-core potential was fitted to the phase shifts of Arndt and MacGregor (AM66). The phases which are given for energies up to 350MeV are fitted by adjusting the parameters in the potential until the calculated phases are the same as those of Arndt and MacGregor within two significant figures in most cases. The potential also fits the low energy scattering data and the deuteron quadrupole moment. The potential fits the phases almost as well as the experimental data fit the phases (R68, p. 6). The potential is given separately for each LSJ state. It has no hard core and is given by the analytic expressions below.

The potentials are in MeV. $x = \mu r$ where $\mu = .7\ \mathrm{fm}^{-1}$ and $\frac{\hbar^2}{M} = 41.47\ \mathrm{MeV\ fm}^2$.

$${}^1S_0 : \quad V = -10.463 \frac{e^{-x}}{x} - 1650.6 \frac{e^{-4x}}{x} + 6484.2 \frac{e^{-7x}}{x}$$

$${}^1D_2 : \quad V = -10.463 \frac{e^{-x}}{x} - 12.322 \frac{e^{-2x}}{x} - 1112.6 \frac{e^{-4x}}{x}$$

$$+ 6484.2 \frac{e^{-7x}}{x}$$

$${}^1G_4 : \quad V = -10.463 \frac{e^{-x}}{x} - 39.025 \frac{e^{-2x}}{x} + 6484.2 \frac{e^{-7x}}{x}$$

$${}^3P_0 : \quad V = -10.463 \left[\left(1 + \frac{4}{x} + \frac{4}{x^2}\right) \frac{e^{-x}}{x} - \left(\frac{16}{x} + \frac{4}{x^2} \right) \frac{e^{-4x}}{x} \right]$$

$$+ 27.133 \frac{e^{-2x}}{x} - 790.74 \frac{e^{-4x}}{x}$$

$$+ 20662. \frac{e^{-7x}}{x}$$

$$^{3}P_{1} \quad : \quad V = 10.463 \left[\left(1 + \frac{2}{x} + \frac{2}{x^{2}}\right) \frac{e^{-x}}{x} - \left(\frac{8}{x} + \frac{2}{x^{2}}\right) \frac{e^{-4x}}{x} \right]$$

$$- 135.25 \frac{e^{-2x}}{x} + 472.81 \frac{e^{-3x}}{x}$$

$$^{3}F_{3} \quad : \quad V = 10.463 \left[\left(1 + \frac{2}{x} + \frac{2}{x^{2}}\right) \frac{e^{-x}}{x} - \left(\frac{8}{x} + \frac{2}{x^{2}}\right) \frac{e^{-4x}}{x} \right]$$

$$- 729.25 \frac{e^{-4x}}{x}$$

$$^{1}P_{1} \quad : \quad V = 31.389 \frac{e^{-x}}{x} - 634.39 \frac{e^{-2x}}{x} + 2163.4 \frac{e^{-3x}}{x}$$

$$^{3}D_{2} \quad : \quad V = - 31.389 \left[\left(1 + \frac{2}{x} + \frac{2}{x^{2}}\right) \frac{e^{-x}}{x} - \left(\frac{8}{x} + \frac{2}{x^{2}}\right) \frac{e^{-4x}}{x} \right]$$

$$- 220.12 \frac{e^{-2x}}{x} + 871. \frac{e^{-3x}}{x}$$

For the coupled states $V = V_C + V_T S_{12} + V_{LS} \vec{L}\cdot\vec{S}$

$$^{3}P_{2} - {}^{3}F_{2} \quad : \quad V_C = \frac{10.463}{3} \frac{e^{-x}}{x} - 933.48 \frac{e^{-4x}}{x} + 4152.1 \frac{e^{-6x}}{x}$$

$$V_T = 10.463 \left[\left(\frac{1}{3} + \frac{1}{x} + \frac{1}{x^{2}}\right) \frac{e^{-x}}{x} \right.$$

$$\left. - \left(\frac{4}{x} + \frac{1}{x^{2}}\right) \frac{e^{-4x}}{x} \right] - 34.925 \frac{e^{-3x}}{x}$$

$$V_{LS} = -2074.1 \frac{e^{-6x}}{x}$$

$$^{3}S_{1} - {}^{3}D_{1} \quad : \quad V_C = - 10.463 \frac{e^{-x}}{x} + 105.468 \frac{e^{-2x}}{x}$$

$$- 3187.8 \frac{e^{-4x}}{x} + 9924.3 \frac{e^{-6x}}{x}$$

$$V_T = -10.463 \left[\left(1 + \frac{3}{x} + \frac{3}{x^2}\right) \frac{e^{-x}}{x} - \left(\frac{12}{x} + \frac{3}{x^2}\right) \frac{e^{-4x}}{x} \right] + 351.77 \frac{e^{-4x}}{x} - 1673.5 \frac{e^{-6x}}{x}$$

$$V_{LS} = 708.91 \frac{e^{-4x}}{x} - 2713.1 \frac{e^{-6x}}{x}$$

In the other states, the one-pion-exchange potential, V_{OPEP}, is employed; alternatively one could use the potential from the highest J state of the same spin and isospin.

$$V_{OPEP} = \frac{10.463}{3} (\vec{\tau}_1 \cdot \vec{\tau}_2) [(\vec{\sigma}_1 \cdot \vec{\sigma}_2) + S_{12} (1 + \frac{3}{x} + \frac{3}{x^2})] \frac{e^{-x}}{x}$$

There are three kinds of integrals that must be evaluated when calculating the matrix elements for the Reid potential, corresponding to terms like $\frac{e^{-\beta x}}{x}$, $\frac{e^{-\beta x}}{x^2}$, $\frac{e^{-\beta x}}{x^3}$. To facilitate the evaluation of these integrals we transform them into repeated integrals of error functions (G61). The integrals correspond to potential shapes given above. For the shape $\frac{e^{-x}}{x}$, we have integral

$$A(n,i,\alpha) = \frac{\lambda}{\pi}^{\frac{2n+1}{2}} \int \rho^{2n-3} \frac{e^{-(\lambda\rho^2 + \sqrt{2}\mu\rho)}}{\sqrt{2}\,\mu} d\vec{\rho}$$

where (2n-2) is the exponent of ρ in Table III-2. In the notation of Chapter III n = 1,2,3,4,5,6,7 corresponds to integrals A,B,C,D,E,F,G respectively. i refers to the

LSJ state as defined in Table III-4. The argument α is dependent on the range parameters, $\alpha \equiv \frac{\mu}{\sqrt{2\lambda}} = \frac{\mu}{\sqrt{2(\lambda_i + \lambda_j)}}$.

We can write the integral as

$$A(n,i,\alpha) = \frac{4}{\mu\sqrt{2\lambda}} \frac{\lambda^{\frac{2n+1}{2}}}{(\sqrt{\lambda})^{2n-1}} e^{\alpha^2} \int_\alpha^\infty (z-\alpha)^{2n-1} e^{-z^2} dz$$

$$A(n,i,\alpha) = \frac{4}{\mu\sqrt{2\lambda}} \frac{\lambda^{\frac{2n+1}{2}}}{(\sqrt{\lambda})^{2n-1}} e^{\alpha^2} \frac{\sqrt{\pi}}{2} (2n-1)!\ i^{2n-1} \operatorname{erfc}(\alpha)$$

i^n $(n \geqslant o)$ is the n^{th} power of the integral operator $i \equiv \int_\alpha^\infty$, so that

$$i^o \operatorname{erfc}(\alpha) = \operatorname{erfc}(\alpha)$$

$$i^n \operatorname{erfc}(\alpha) = \int_\alpha^\infty i^{n-1} \operatorname{erfc}(t)\, dt$$

For shape $\frac{e^{-x}}{x}$, $A(n,i,\alpha) = \frac{1}{\alpha} M_{2n-1}(\alpha)$

For shape $\frac{e^{-x}}{x^2}$, $A(n,i,\alpha) = \frac{1}{2\alpha^2} M_{2n-2}(\alpha)$

For shape $\frac{e^{-x}}{x^3}$, $A(n,i,\alpha) = \frac{1}{4\alpha^3} M_{2n-3}(\alpha)$

where $M_n(\alpha) = \sqrt{\pi}\ e^{\alpha^2}\ n!\ i^n \operatorname{erfc}(\alpha)$.

It can be shown that for the more general potential shapes, the expressions are only slightly modified.

For shape $\frac{e^{-\beta x}}{x}$, $A(n,i,\beta\alpha) = \frac{1}{\alpha} M_{2n-1}(\beta\alpha)$

For shape $\frac{e^{-\beta x}}{x^2}$, $A(n,i,\beta\alpha) = \frac{1}{2\alpha^2} M_{2n-2}(\beta\alpha)$

For shape $\frac{e^{-\beta x}}{x^3}$, $A(n,i,\beta\alpha) = \frac{1}{4\alpha^3} M_{2n-3} (\beta\alpha)$.

The Bressel Potential

The Bressel potential is derived from the Hamada-Johnston potential (HJ62) by replacing the infinite repulsive cores by finite cores of different heights in different states. The Hamada-Johnston potential is of the form

$$V = V_C + V_T S_{12} + V_{LS} \vec{L}\cdot\vec{S} + V_{LL} L_{12}$$

where C, T, LS, and LL refer to central, tensor, linear $\vec{L}\cdot\vec{S}$ and quadratic $\vec{L}\cdot\vec{S}$ potentials, respectively. L_{12} is the operator defined

$$L_{12} = \{\delta_{LJ} + (\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(2)})\} L^2 - (\vec{L}\cdot\vec{S})^2$$

V_C, V_T, V_{LS}, and V_{LL} are given by

$$V_C = .08 \left(\frac{m}{3}\right) (\vec{\tau}^{(1)}\cdot\vec{\tau}^{(2)})(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(2)}) Y(x)[1 + a_c Y(x) + b_c Y^2(x)]$$

$$V_T = .08 \left(\frac{m}{3}\right) (\vec{\tau}^{(1)}\cdot\vec{\tau}^{(2)})(\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(2)}) Z(x)[1 + a_t Y(x) + b_t Y^2(x)]$$

$$V_{LS} = m G_{LS} Y^2(x) [1 + b_{LS} Y(x)]$$

TABLE V-1

Parameters of the Kerman-Bressel Potential

Core Heights

State		T	S	$V_C^{T,S}$	$V_T^{T,S}$	$V_{LS}^{T,S}$	$V_{LL}^{T,S}$
Singlet	even	1	0	670			- 46
Triplet	odd	1	1	670	-50	-374	332
Triplet	even	0	1	467	99	-157	224
Singlet	odd	0	0	468			- 46

TABLE V-2

Parameters of the Kerman-Bressel Potential

Potential Parameters

State		T	S	a_C	b_C	a_T	b_T	G_{LS}	b_{LS}	G_{LL}	a_{LL}	b_{LL}
Singlet	even	1	0	8.7075	10.6						.2	-.2
Triplet	odd	1	1	-11.2	3.28	-1.29	.55	.1961	-7.12	-.000891	-7.26	6.92
Triplet	even	0	1	6.0	-1.0	-.5	.2	.0743	-.1	.00267	1.8	-.4
Singlet	odd	0	0	-8.0	12.0					-.00267	2.0	6.0

$$V_{LL} = m\, G_{LL} \, \frac{Z(x)}{x^2} \, [1 + a_{LL} \, Y(x) + b_{LL} \, Y^2(x)]$$

where m is the pion mass, $Y(x) = \frac{e^{-x}}{x}$, and

$$Z(x) = (1 + \frac{3}{x} + \frac{3}{x^2}) \, Y(x)$$

x is measured in terms of pion Compton wavelengths

x_C (core radius) = .4852 meson Compton wavelengths. The core heights are given in Table V-1. The meson mass was adjusted by Bressel for the three states $T = 1 \, (\substack{nn \\ pp})$, $T = 1$ (np), and $T = o$ (np) giving 137.11, 133.08, 137.34MeV respectively. Charge symmetry is preserved but this potential is not charge independent. Some of the Hamada-Johnston potential parameters were amended and the latest parameters are given in Table V-2. The potential was fitted directly to a set of experimental data ranging in energy from 0 to 350MeV. Since additional parameters are used as compared to Hamada-Johnston, the fit is bound to be superior.

In our calculation we wish to work with a charge independent potential. We take, therefore, a weighted average for the meson mass in the T=1 state.

For T=o , m = 137.34MeV $\mu = .69601615 \text{ fm}^{-1}$

For T=1 , m = 135.77MeV $\mu = .68804275 \text{ fm}^{-1}$

As for the Reid potential, we must evaluate the matrix elements which turn into integrals of the type

$$A(j,i,\lambda) = \frac{\lambda^{\frac{2j+1}{2}}}{\pi} \int \rho^{2(j-1)} \, e^{-\lambda\rho^2} \, V_i(\rho) \, d\vec{\rho}$$

Only the last argument of the A differs from the A defined for the Reid potential. The α and λ are related through the equation $\alpha = \frac{\mu}{\sqrt{2\lambda}}$. We can write this as integrals corresponding to the soft core region plus integrals over the remaining region. If c is the core radius, and $V_{c,i}$ the core height in the i^{th} state,

$$A(j,i,\lambda) = 4\lambda^{\frac{2j+1}{2}} V_{c,i} \int_0^c \rho^{2j} e^{-\lambda\rho^2} d\rho + 4\lambda^{\frac{2j+1}{2}} \times \int_c^\infty \rho^{2j} e^{-\lambda\rho^2} V_i(\rho) d\rho$$

The second integral we evaluate numerically; the first integral can be expressed as an incomplete gamma function, which in turn can be expressed as a confluent hypergeometric function (AS64, pp. 260-262). Then we write

$$A(j,i,\lambda) = 4\lambda^{\frac{2j+1}{2}} V_{c,i}\, c^{2j+1} \left(\frac{1}{2j+1} + \frac{z}{2j+3} + \frac{z^2}{(2j+5)2!} + \frac{z^3}{(2j+7)3!} + \cdots \right) + 4\lambda^{\frac{2j+1}{2}} \int_c^\infty \rho^{2j} e^{-\lambda\rho^2} V_i(\rho) d\rho$$

where $z = -\lambda c^2$

The Pease-Feshbach Potential

For comparison with other people's work, we use the potential of Pease and Feshbach (PF52). It is potential #3 in Table II of that paper. The potential has the form

$$V = -V_o \{[1 - \frac{1}{2} g + \frac{1}{2} g \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)}] f(\frac{r}{r_c}) + \gamma S_{12} f(\frac{r}{r_t})$$

where $f(x) = \frac{e^{-x}}{x}$

The constants in the potential are

$V_o = 46.96$ MeV

$g = .005$

$\gamma = .5085$

$r_t = 1.70$

$\frac{r_t}{r_c} = 1.44$

This potential fits the deuteron binding energy, the deuteron quadrupole moment, the singlet scattering length and effective range, and the triplet effective range. This potential we write in the same form as the Reid potential, so that the matrix elements can be evaluated the same way.

Singlet states: $V = -38.42 \frac{e^{-1.21008\mu r}}{\mu r}$ with $\mu = .7$

Triplet states: $V = -38.81 \frac{e^{-1.21008\mu r}}{\mu r}$

$$-28.4162 \, S_{12} \frac{e^{-.84034\mu r}}{\mu r}$$

This potential is attractive, and consequently it should be much easier to find a good trial function since we need not build in the trial function correlation due to short range repulsion.

The Coester-Yen Potential

The last potential is one developed by Coester and Yen (CY63). This is a spin-dependent central Serber potential whose volume integral is zero. The feature that makes it suitable for our purposes is that it has a soft repulsive core as well as an attractive part, both of Yukawa shape. It predicts the low energy scattering parameters and fits roughly the Yale phase shifts (BHLP60) for the S and D states. The potential has the form $V = V_o\ (4e^{-2\mu r} - e^{-\mu r})/\mu r$ with parameters given in Table V-3.

TABLE V-3

S	V_o (MeV)	μ/m_π
0	2126	2.81
0	2307	2.92*
1	3991	3.26

where $m_\pi = 1.413$ fermis.

*These parameters are used in the present calculation.

CHAPTER VI

NUMERICAL CALCULATIONS AND THEIR INTERPRETATIONS

The Rayleigh-Ritz variational calculation gives an upper bound of the ground state energy by varying the parameters in the trial function until a minimum of the energy is found. In this way one acquires the lowest upper bound of the ground state energy that can be obtained within the class of trial functions employed. The difference between the actual ground state and the upper bound is smaller the closer the variational wave function is to the actual wave function. However, since the lowest upper bound is stationary for the parameters in the trial function, the difference in energies is an infinitesimal of higher order than the difference between the actual and variational wave functions (M62, chapter 18). A good check on a trial function that gives a reasonable upper bound on the energy is to use it to calculate other physical observables. In our case we calculate the mass radius of the triton and the D-state probability. The latter quantity, however, is even more uncertain in the triton than in the deuteron (P62, chapter 5.1) because one would expect the exchange effects to be enhanced by the smaller size of the triton. Estimates anywhere between 2% to 8% should not be considered inconsistent with experiment.

General Procedure of Performing the Minimization

In the present calculation one can distinguish between two kinds of minimization. A minimum can be found by varying the linear parameters only by the matrix diagonalization technique described in Chapter IV. One then assumes the non-linear parameters to be fixed. In the second kind of minimization, one varies the non-linear parameters also and performs a linear parameter minimization for each set of non-linear parameters in the non-linear parameter search process. In this way all the parameters are varied. Whenever we refer to "minimization with respect to the parameters" we mean it in the latter sense, i.e. a minimization with respect to both the linear and non-linear parameters.

In general, when we minimize some quantity, irrespective of whether it be the energy, force factor, or ε, we follow the procedure that we outline below. We initially determine the state that will dominate the overall wave function, either by general arguments about the relative magnitudes of potential and kinetic energy, or by trial and error. Whether we have found the dominant state or not, will become evident when we calculate the amplitudes of the component states in the overall wave function.

We calculate the quantity that we wish to minimize using two or three non-linear parameters in the dominant state. Our initial choice of input values for the non-linear parameters is based on certain physical considerations. The root-mean-square radius of a Gaussian with range parameter λ is $\sqrt{\frac{3}{2\lambda}}$. When we take the triton radius, i.e. 1.7 fm., to be the approximate size of the distribution we use $\lambda_i \simeq .25\ \mathrm{fm}^{-2}$ as one range parameter. We then need one or more larger parameters for short range cancellation when we have a repulsive core and one or more small parameters to pick up the longer range attraction of the potential. It is impossible, however, to simulate $e^{-\alpha\rho}$ behaviour with a sum of Gaussians for large ρ. It turns out that non-linear parameters found by searching for a minimum will have values by and large between .05 and 5. indicating that the search routine finds parameters of the order of magnitude that we expect.

After we have made our initial choice of the number and values of the non-linear parameters, we minimize with respect to these. We then add one non-linear parameter at a time, and minimize with respect to all of them to obtain a new minimum. When the addition of a new parameter has negligible effect on the minimum, i.e. of the order of 1% or less, we stop adding more parameters. Having obtained the number of non-linear parameters we need in the dominant state, we use an equal number of parameters in each of the other states. The parameters in each of the other states are determined by leaving the non-linear parameters in the dominant state fixed and varying the parameters of the additional state to obtain a minimum. This is done for each state in turn so that we end up with a set of non-linear parameters for each state. With the non-linear parameters so obtained, we minimize with respect to the linear parameters to obtain the final result. Ideally, one should do a variation of the non-linear parameters also but this would take too long even on modern high-speed computers. The approximation, however, is not as bad as it seems. In the case of the Pease-Feshbach potential we do a variation with three states according to this procedure. After we have found the minimum in this way, we start with the parameters for this minimum and continue to vary all the parameters. The increase in binding energy turns out to be less than 1%.

Initially we are interested only in an approximate value for the minimum which may differ from the precise minimum by as much as 5%. This is true throughout for the force factor and ε. We therefore minimize until the approximate minimum changes by less than 1%. Minimizing until the parameters have this accuracy would require many more passes. We feel that this is not necessary except when doing the final minimization of the energy so that the most accurate wave function can be found. The radius and component-state probabilities are calculated only as a final calculation.

When we are searching for the minimum, it is possible that the minimization procedure might want to evaluate the function for parameters which include one or more negative λ_i's. This is, of course, an unphysical region in parameter space, and the integrals for the matrix elements diverge. To prevent having to deal with negative λ_i's we transform the parameter space into one in which the effective parameters are $\lambda_i' = \frac{1}{\sqrt{\lambda_i}}$. The square root reduces the difference between the parameters so that the same increments can be used for all parameters, and the reciprocal ensures that as the effective parameter λ_i' is increased, λ_i will approach zero but will never become negative. Another effective way of searching for a minimum which does have the possibility of looking at parameters which are negative, but it never has in our experience, is to work in a parameter space which has the same parameter directions as the actual parameters but the parameters are scaled down by the magnitude of the input parameters, i.e. $\lambda_i' = \frac{\lambda_i}{\lambda_i \text{ input}}$. If one takes a range of input parameters between .1 and 5 with increments of .05 in the search procedure, one finds that the parameters do not become negative under normal circumstances. It must be remembered that before calculating the matrix elements we must apply the inverse transformation on the parameters and after calculating the energy we must transform back to the parameter space in which the searching is done.

The matrix elements are calculated using the expressions given in Chapter III. We need matrix elements for the normalization, kinetic energy, and the potential energy. When we calculate ε we have to write separate matrices for the repulsive and attractive part of the potential energy. For the Pease-Feshbach, Coester, and Reid potentials we use the closed expressions given in Chapter V. The repeated integrals of the error functions are evaluated in three domains. When $\alpha \leqslant .5$ a power series expansion is used

$$i^n \operatorname{erfc}(\alpha) = \sum_{k=o}^{\infty} \frac{(-1)^k \alpha^k}{2^{n-k}\, k!\; \Gamma(1 + \frac{n-k}{2})}$$

with terms corresponding to $k = n+2, n+4, \ldots$ being zero. For arguments of this order of magnitude, the series converges very rapidly and no subtracting of big numbers occurs to give a small result, which is the case when $\alpha > 1$. The repeated integrals of the error functions are regular solutions of the differential equation

$$\frac{d^2y}{d\alpha^2} + 2\alpha \frac{dy}{d\alpha} - 2ny = o \qquad (1)$$

The following recurrence relation exists (G61)

$$i^n \operatorname{erfc}(\alpha) = -\frac{\alpha}{n}\, i^{n-1} \operatorname{erfc}(\alpha) + \frac{1}{2n}\, i^{n-2} \operatorname{erfc}(\alpha) \qquad (2)$$

In order to calculate $i^k \operatorname{erfc}(\alpha)$ we can generate the sequence $w_v^n(\alpha)$, $(v=n, n-1, \ldots, 1, 0, -1)$ starting with $w_{n+2}^n(\alpha) = o$, $w_{n+1}^n(\alpha) = 10^{-30}$ and using relation (2) for the remaining members in the sequence. Gautschi (G61) has shown that

$$\lim_{n\to\infty} \frac{w_k^n(\alpha)}{w_{-1}^n(\alpha)} = \frac{\sqrt{\pi}}{2}\, e^{\alpha^2}\, i^k \operatorname{erfc}(\alpha) \qquad (\alpha > o).$$

In order to obtain accuracy of 1 part in 10^8 we use the relation

$$v \geqslant \left(\frac{2\sqrt{2N}\,\alpha + 8 \ln 10 + \ln 2}{2\sqrt{2}}\right)^2$$

where N is the largest k we have to evaluate, i.e. N=13. For $\alpha=5$, $v \geqslant 25$ will give such an accurate result. As α increases v becomes smaller, but as α decreases v becomes large. It is more efficient therefore to calculate a table of values of the repeated integrals of the error function for a range of arguments lying between .5 and 5, and then to interpolate in order to obtain the value at the required argument. It turns out that

$$f_n(\alpha) = n!\, e^{x^2} \sqrt{\pi}\; i^n \operatorname{erfc}(\alpha)$$

is a monotonically slowly decreasing function. We calculate $i^n \operatorname{erfc}(\alpha)$ by integrating the differential equation (1) from $\alpha=5$ to $\alpha=.5$. The initial boundary conditions are obtained by using the method of the recurrence relation outlined above, and noting that

$$\frac{d}{d\alpha}\ i^n\ \mathrm{erfc}(\alpha) = -i^{n-1}\ \mathrm{erfc}(\alpha) \qquad n=o,\ 1,\ 2,\ldots$$

The functions $f_n(\alpha)$ were tabulated for $n=1,\ldots,13$ and for $\alpha=.5$ to 5. with steps of .05. For the interpolation we used Aitken's method and fitted a sixth order polynomial to the six nearest values in the table. Near the values $\alpha=.5$ and $\alpha=5.$ adjustments were made so that the interpolation process used the end point and the nearest five inside the domain (AS64, p. 879).

No closed expression can be obtained for the Bressel potential matrix elements, and therefore we use the series expansion of the integral for the core region and use Simpson's rule outside this region. The number of intervals and the distance of the integration is determined by the accuracy of the integral that is required. We integrate to the distance in which the magnitude of the integrand has fallen to 10^{-8} of its maximum value, and we keep doubling the number of steps until the value of the integral changes by less than 10^{-4}.

The diagonalization of the matrices is done by the Jacobi method as written up by Greenstadt (RW59, chapter 7). The computer code was available in the subroutine library of the McMaster computers and was called from there whenever it was needed.

Pease-Feshbach Potential

The Pease-Feshbach potential is attractive everywhere. It is expected that the symmetric S-state of the type Ψ_1 is most effective in binding the triton with this potential. Ψ_1 has less curvature and consequently less kinetic energy associated with it than the other symmetric S-states, Ψ_5, Ψ_6, Ψ_8, and Ψ_{10}. Furthermore, it can take greater advantage of the attraction at zero interparticle distance than states like Ψ_5, Ψ_6, and Ψ_8 that vanish when ρ is zero. It is not difficult to obtain binding with Ψ_1. In Table VI-1 we give the results when we include four, five or six terms and minimize the energy until the parameters are constant to within .0001. This usually takes a relatively large number of passes, i.e. of the order of ten for four terms, depending on the initial choice of the parameters. It is seen from Table VI-1 that the energy changes very little as we increase the number of parameters. The small change in energy is about 1% of the final energy that we obtain when we use all the states. We feel, therefore, justified that for a calculation such as this one which is designed to test the wave function we use only four parameters per state. These four parameters are varied until the energy minimum does not change by more than 1%. That the difference between the two methods is not very great is evident from Table VI-2 where we have similar results as in Table VI-1 except we minimize the energy until a change of less than 1% in the energy occurs in one pass. The fact that the five parameter case does not produce as low an energy as the four parameter case should not be alarming because the difference is less than 1%.

In Table VI-3 we list the energies obtained as we add four terms of another state and vary the nonlinear parameters of the added state only; all the linear parameters are varied each time the energy is evaluated. The trends are very clear from this arrangement of energies. The relative importance of each state is indicated by the amount that the additional state increases the binding energy. If the vectors $\vec{\rho}$ and $\vec{r}$ have angular momentum assigned to them, it is expected that the ℓ=o state for both vectors would be the lowest state of the system. We write this as ss. The first s refers to the angular momentum associated with $\vec{\rho}$, the second s to the angular momentum associated with $\vec{r}$. We can write down such constituents of the states in our work.

$\Psi_1 \sim$ ss

$\Psi_2 \sim$ ss, pp

$\Psi_3 \sim$ pp

$\Psi_4 \sim$ sd, ds, pp

$\Psi_5 \sim$ ss, dd

$\Psi_6 \sim$ ss, dd, gg

$\Psi_7 \sim$ sd, ds, pp, pf, fp, ff

$\Psi_8 \sim$ ss, dd, gg, ii

$\Psi_9 \sim$ ss, pp, dd, ff

$\Psi_{10} \sim$ ss

Since Ψ_5 has a definite ratio of ss and dd components, it will not bind the triton but since Ψ_1 is pure ss it does. For the same reason Ψ_5 is more effective in increasing the binding than Ψ_6 or Ψ_8 and Ψ_4 is more effective than Ψ_7. One would expect Ψ_{10} to have more influence since it is also a symmetric S-state with the lowest possible excitation of the $\vec{\rho}$ or $\vec{r}$ vectors. There may be two reasons for its apparent ineffectiveness. In the first place, it has more kinetic energy associated with it than does Ψ_1, and secondly this function can be approximated by a pair of functions of the type found in Ψ_1, i.e.

$$(\rho^2+r^2)\ e^{-\lambda(\rho^2+r^2)} = -\frac{d}{d\lambda}\ e^{-\lambda(\rho^2+r^2)}$$

$$\sim \frac{-e^{-(\lambda+\Delta\lambda)(\rho^2+r^2)} + e^{-\lambda(\rho^2+r^2)}}{\Delta\lambda}$$

for $\Delta\lambda$ small. Any two terms in Ψ_1 with range parameters which are almost equal and coefficients which are equal but opposite in sign will give a term of the type found in Ψ_{10}. If functions of the latter type are desirable in the calculation, the search procedure will adjust the parameters of Ψ_1 in such a way as to simulate a term of

Ψ_{10}. Functions of the type Ψ_5 seem to have more effect on the binding because they have different shape, and no simple relation exists between Ψ_1 and Ψ_5 as did between Ψ_1 and Ψ_{10}. Furthermore, Ψ_5 does introduce D-state two-body forces in the problem which help in the binding of the triton.

If we do a linear parameter minimization only with the range parameters found for Ψ_1, Ψ_4, and Ψ_5, we obtain an energy of -4.219MeV. If we minimize further with respect to the non-linear parameters we obtain a decrease in the energy of less than 1%. We feel, therefore, that the approach of using all the non-linear parameters that have been obtained systematically and minimize them with respect to the linear parameters only is justified. The final result of the Pease-Feshbach calculation is given in Table VI-4. Using the range parameters of states Ψ_1, Ψ_4, Ψ_5, Ψ_6, Ψ_7, Ψ_8, Ψ_{10} we obtain a force factor equal to 1.077 with binding of 8.5MeV.

Although this calculation employs more free parameters in the trial function and includes more states than the Pease-Feshbach calculation (PF52), the energy that we obtain is higher than the energy that they calculated, i.e. -8.48MeV. Blatt et al. (BDL62) have been able to obtain upper bounds on the energy of the triton with the Pease-Feshbach potentials which are about 1MeV lower than those obtained by Pease and Feshbach themselves.

Thus Blatt et al. get about 9.5MeV binding which is almost twice as much as we obtain. They do use a more elaborate wave function and more states. Even with a longer more accurate parameter search, we could not hope to come close to their binding energy. In fact, we have to increase the potential strength by more than 8% to come close to the value for binding that Blatt et al. obtain. Their estimate of the Coulomb radius is about 25% smaller than that calculated from the observed Coulomb energy in He^3. The discrepancy of Pease and Feshbach (PF52) is even greater. The radius that we obtain when compared to an estimate of the mass radius of point particles in the triton, is about 10% too small. The percentage D-state is the same within the relatively large uncertainty limits that we have placed on it.

The conclusion that we have to reach concerning the method is that the trial function we use is not as good as the one of Pease and Feshbach or the one used by Blatt et al. In both of the latter calculations trial functions with exponential decay for large interparticle distance are used whereas our functions decay like Gaussian functions, and therefore not enough of the long range attraction of the potential is felt. The tensor force contribution to the energy is calculated to the same proportion as in the other calculations since the D-state probabilities are the same.

If we would want to make improvements on our trial function, the symmetric S-state would stand in need of the greatest modification. This conclusion will become even more evident from the calculations with the other potentials. The fact that we obtain a larger radius than the previous calculations is also due to the superposition of Gaussians in the trial function. The Yukawa shape of the potential gives a faster increase in the strength of the potential as the interparticle distance becomes smaller. The superposition of exponentials in a wave function can also yield a faster increase in amplitude as the interparticle distance becomes smaller. The amplitude of the sum of Gaussians increases more slowly for smaller interparticle distances and there is, in fact, a decrease in amplitude when the Gaussian is multiplied by ρ^2, ρ^4, ... This is due to the fact that Gaussians have zero slope at the origin whereas the exponential function has slope equal to its decay constant. For the Yukawa shape of the potential a sum of Gaussians tends to pick up a greater proportion of the attraction in the intermediate region than the superposition of exponentials which picks up most of the attraction at small interparticle distances. This explains the relatively large radius that we have obtained. It is noteworthy that the 8% deviation of the force factor from unity is equal to the fraction of potential energy that is needed in order to give experimental binding energy.

TABLE VI-1

Minimizing the Energy with the Pease-Feshbach Potential

Energy (MeV)	State	Number of Range Parameters	Range Parameters
-.891431 MeV	Ψ_1	4	.037969
			.155283
			.553344
			2.209480
-.934747 MeV	Ψ_1	5	.025930
			.097282
			.311559
			.991558
			3.799778
-.945459 MeV	Ψ_1	6	.017321
			.058478
			.170384
			.476221
			1.414916
			5.326559

The energy is minimized by varying the parameters until the parameters do not change by more than .0001.

TABLE VI-2

Minimizing the Energy with the Pease-Feshbach Potential

Energy	State	Number of Range Parameters	Range Parameters
-.6683	Ψ_1	3	.078593
			.310427
			1.240213
-.8363	Ψ_1	4	.062593
			.949900
			.268458
			3.788709
-.8345	Ψ_1	5	.065689
			.271775
			.943609
			2.478820
			7.241909

The energy is minimized by varying the parameters until a change of less than 1% of the energy occurs in one pass of the minimization.

TABLE VI-3

Energies Obtained with the Pease-Feshbach Potential

Energy (MeV)	States	Type of State Added
- .836	Ψ_1	-
- .836	Ψ_1, Ψ_2	mixed symmetry S-state
- .836	Ψ_1, Ψ_3	symmetric P-state
-3.614	Ψ_1, Ψ_4	symmetric D-state
-1.530	Ψ_1, Ψ_5	symmetric S-state, $(\vec{\rho}\times\vec{r})^2\ \Psi_1$
-1.236	Ψ_1, Ψ_6	symmetric S-state, $(\vec{\rho}\times\vec{r})^4\ \Psi_1$
-2.839	Ψ_1, Ψ_7	symmetric D-state, $(\vec{\rho}\times\vec{r})^2\ \Psi_4$
-1.071	Ψ_1, Ψ_8	symmetric S-state, $(\vec{\rho}\times\vec{r})^6\ \Psi_1$
- .836	Ψ_1, Ψ_9	mixed symmetry S-state, $(\vec{\rho}\times\vec{r})^2\ \Psi_2$
- .934	Ψ_1, Ψ_{10}	symmetric S-state, $(\rho^2+r^2)\Psi_1$

The basic Ψ_1 state is the one with the second set of parameters in Table VI-2. The non-linear parameters of the additional state and all the linear parameters are varied to give a minimum.

TABLE VI-4

Minimization of the Energy with the Pease-Feshbach Potential with Respect to the Linear Parameters Only

Non-linear Parameters

State	Parameters			
Ψ_1	.065293	.949900	.268458	3.788709
Ψ_2	.116651	.405457	1.206929	3.553610
Ψ_3	.070648	.340306	3.748565	2.179583
Ψ_4	.083253	1.060123	.341373	3.910593
Ψ_5	.090107	.487312	.181185	1.696295
Ψ_6	.053228	.754226	.195304	2.329725
Ψ_7	.083684	1.380015	.503073	3.990299
Ψ_8	.068727	1.027624	.268458	2.957207
Ψ_9	.117906	.466435	1.331884	4.388597
Ψ_{10}	.031624	.474113	.153030	1.897196

Linear Parameters

State	Parameters			
Ψ_1	.299246	.381735	.810426	.049152
Ψ_2	.007624	.011769	.005860	.001564
Ψ_3	.007032	.043550	-.002000	.019157
Ψ_4	-.016340	-.023534	-.028916	-.009329
Ψ_5	-.022878	-.109002	-.025983	-.036144
Ψ_6	.028832	.240685	.046219	.087046
Ψ_7	.006604	-.030707	-.032506	-.016439
Ψ_8	-.025693	-.091354	-.014399	-.036327
Ψ_9	-.001524	.000657	.001904	.000760
Ψ_{10}	.012829	.018835	.069923	-.000279

Energy = -4.7919 MeV

Kinetic Energy = 42.1651 MeV

Potential Energy = -46.9570 MeV

R_{rms} = 1.56 fm.

$P_S = 96.76\%$

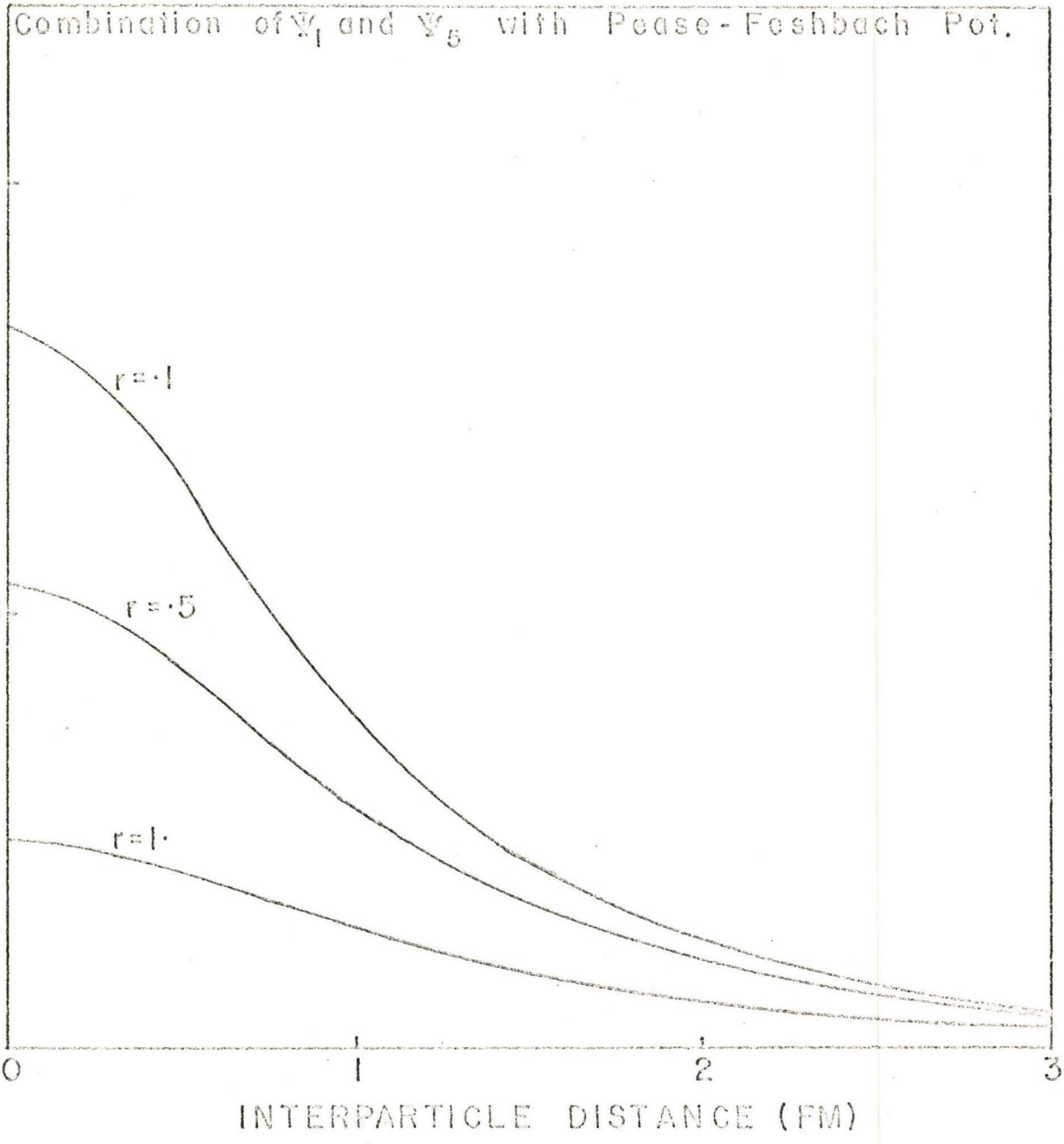
$P_{S'} = .15\%$

$P_P = .24\%$

$P_D = 2.86\%$

Figure VI-1

Graph of the Angular-Averaged Wave Function for Pease-Feshbach Potential

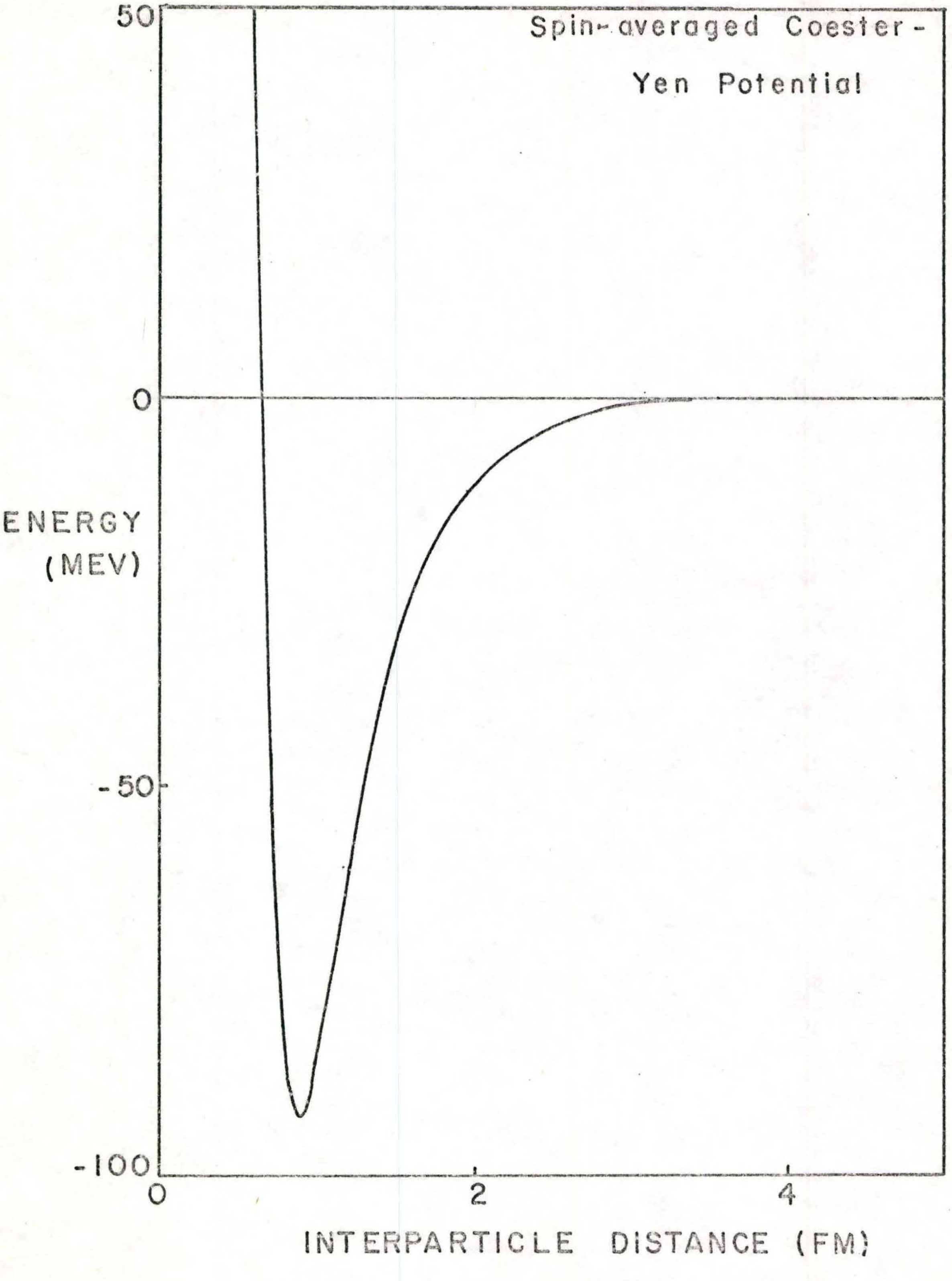


The Coester-Yen Potential

The calculations with the Pease-Feshbach potential indicate that the Gaussian type wave functions are unable to produce the binding that exponential wave functions will give. We subsequently did a calculation with the Coester-Yen potential, which has a soft core, to see how results with the Gaussian-shaped trial functions compared to the results obtained when exponential trial functions are used.

Although the Coester-Yen potential is spin-dependent, we make the approximation that the force bond between a pair of particles in the triton is $1/2(V_{t,e} + V_{s,e})$ regardless of the two-body spin-state (BW52, p. 195). We have sketched the spin-averaged potential in Figure VI-2. With such a potential we can obtain results only with the symmetric S-state and therefore states Ψ_1, Ψ_5, Ψ_6, Ψ_8 and Ψ_{10} are used in this calculation. These states have only even two-body angular momentum components because of the total symmetry of the spatial part of these functions. When we calculate the energy directly, we obtain no binding with our usual set of the Gaussian type wave functions. Thus, we proceeded with the force factor. The results are tabulated in Table VI-5. The force factor is negative when either state Ψ_1 or state Ψ_{10} is included. This is understandable since both these states have relatively large amplitude at the origin where the repulsive part of

Figure VI - 2


Spin-averaged Coester-
Yen Potential
50
0
-50
-100
ENERGY
(MEV)
0
2
4
INTERPARTICLE DISTANCE (FM)

the potential is strongest. Ψ_5 is the dominant state since it is zero at the origin and has the least amount of internal excitation of those states that are zero at the origin.

We follow the same procedure as with the Pease-Feshbach potential to obtain the non-linear parameters in states Ψ_5, Ψ_6, and Ψ_8, except that in the Pease-Feshbach case the energy is minimized whereas in this case the force factor, γ, is minimized. For states Ψ_1 and Ψ_{10} we obtain the non-linear parameters by minimizing the energy of the system with the potential multiplied by the force factor found using Ψ_5 only. The results are given in Table VI-6. If we do a linear parameter minimization of the force factor using the non-linear parameters of Ψ_5, Ψ_6, and Ψ_8, we obtain a force factor of 1.4152. Using all the non-linear parameters that we have obtained so far, we minimize the energy with respect to the linear parameters when $\gamma=1.4$. The results are tabulated in Table VI-7. The angular-averaged wave function is drawn in Figure VI-3 for three values of $r=|\vec{r}|$.

In order to be able to compare the results for different force factors with similar results of calculations with the exponential trial functions, we obtained a set of values for the potential, kinetic, and binding energy for different γ. The variation of these quantities

Figure VI-3

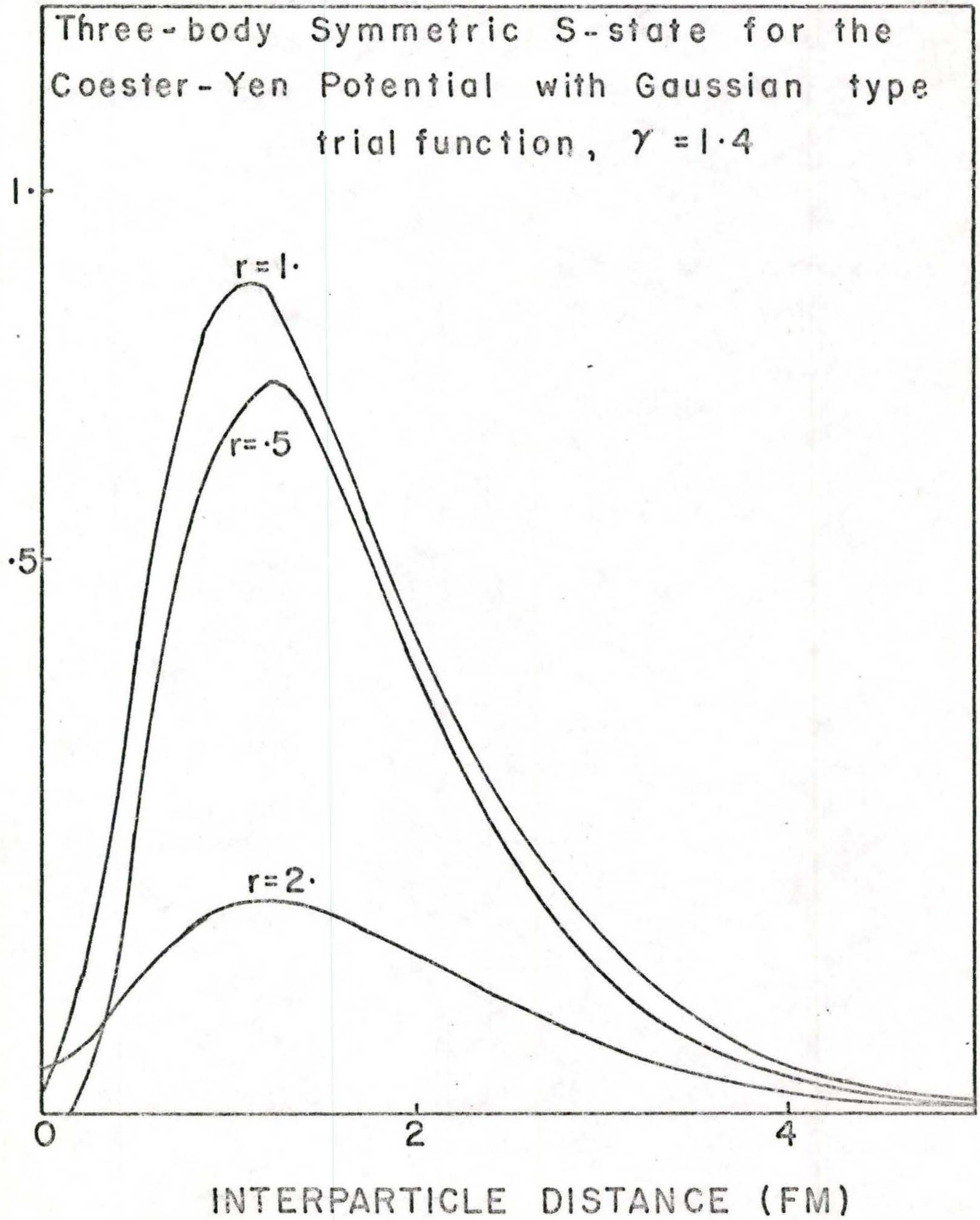
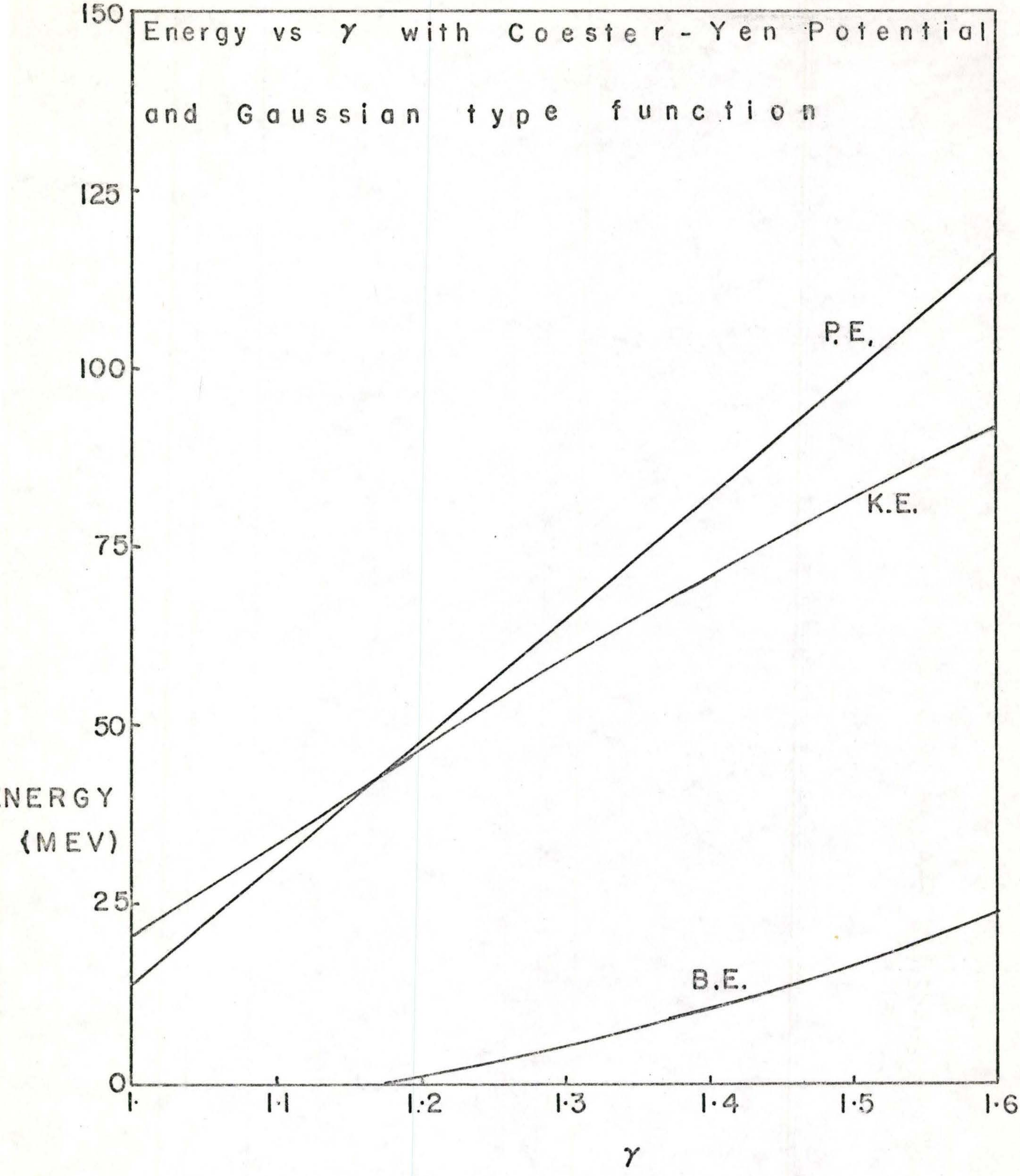

Three-body Symmetric S-state for the Coester-Yen Potential with Gaussian type trial function, $\gamma = 1\cdot4$
1·
·5
r=1·
r=·5
r=2·
0
2
4
INTERPARTICLE DISTANCE (FM)

Figure VI - 4


Energy vs γ with Coester - Yen Potential and Gaussian type function
150
125
100
75
50
25
0
NERGY (MEV)
P.E.
K.E.
B.E.
1·
1·1
1·2
1·3
1·4
1·5
1·6
γ

with respect to γ is shown in Figure VI-4.

The calculation of the binding energy of the triton with the Coester-Yen potential was done also with a different trial function. The new trial function assumed the form

$$\Psi = f(r_{12})\ f(r_{23})\ f(r_{31})$$

where $f(r) = \frac{1}{\sqrt{r}} \sum_{i=o}^{k} c_i\ e^{-\lambda_i r}$ with $\sum_{i=o}^{k} c_i = o$. This form of trial function was chosen because it falls off like an exponential function at large distances. The factor $\frac{1}{\sqrt{r}}$ is inserted because van Wageningen and Kok (VK67) found that exponential trial functions of this type multiplied by r^{-n} gave the best results in a triton calculation when $n \simeq 1/2$. The sum of the coefficients is zero to ensure that the wave function is zero for zero interparticle distance.

We have derived formulae for the potential and kinetic energy using this trial function in Appendix B. We search for a minimum in the energy using the non-linear parameter search routine (M67) for all the parameters. The decay constants of the exponentials are all free parameters, but the coefficients have certain conditions imposed on them, depending on how we wish to suppress the wave function at the origin. One condition on the coefficients determines the normalization, another that $f(o)=o$.

It turns out that we are unable to obtain binding with only two terms in f(r). In this case, we have only two free parameters with respect to which we minimize the energy. With three terms and the condition that f(o) = f'(o)=o, we arrived at some binding as indicated in Table VI-7A The f'(o)=o condition prevents the function from increasing too quickly near the origin. When we set f"(o)=o in the case of four parameters we do get a substantial increase in binding. The reason that, when we use five terms and the additional condition of f'''(o)=o, we do not obtain as much binding is that the function rises too slowly near the origin and does not feel all the attraction of the potential. We therefore relax the condition f'''(o)=o and use the additional degree of freedom to vary one of the coefficients. Since we obtain an increase in binding of only .5MeV in the two best calculations, we feel that the further addition of terms will not increase the binding appreciably. The final results of the calculation are

Energy = - 7.296 MeV
Kinetic Energy = 37.240 MeV
Potential Energy = -44.536 MeV
$R_{r.m.s.}$ = 1.67 fm
$R_{Coulomb}$ = 2.39 fm

Within the approximations of this simplified calculation, the results agree well with the experimental values (the

Coulomb radius, calculated from the Coulomb energy in He^3 with the assumption that the charge is distributed uniformly throughout a sphere of radius $R_{Coulomb}$, is 2.3 fm (D64, p. 69)). Figure VI-5 is a graph of f(r); the behaviour of this wave function as a function of r is independent of the position of the third particle.

We did the same calculation for several values of the force factor in order to study the behaviour of the potential, kinetic, and binding energy as γ varies. The results are shown graphically in Figure VI-6. When this graph is compared to Figure VI-4, it is seen that the exponential function gives consistently better results for all γ. The difference in the binding energy which is seen in the two graphs must be attributed completely to the different trial functions used since the potential is the same in both instances. In order to be able to predict the correction that must be applied to the binding energy calculated with the Gaussian type wave function, we have plotted the uncorrected binding versus the correction as obtained from graphs VI-4 and VI-6. This graph (Figure VI-7) turns out to be nearly a straight line. This correction may be thought of as being independent of the potential used but dependent only on the fact that one calculation is done with a superposition of Gaussians whereas the other with a superposition of exponentials.

Figure VI-5

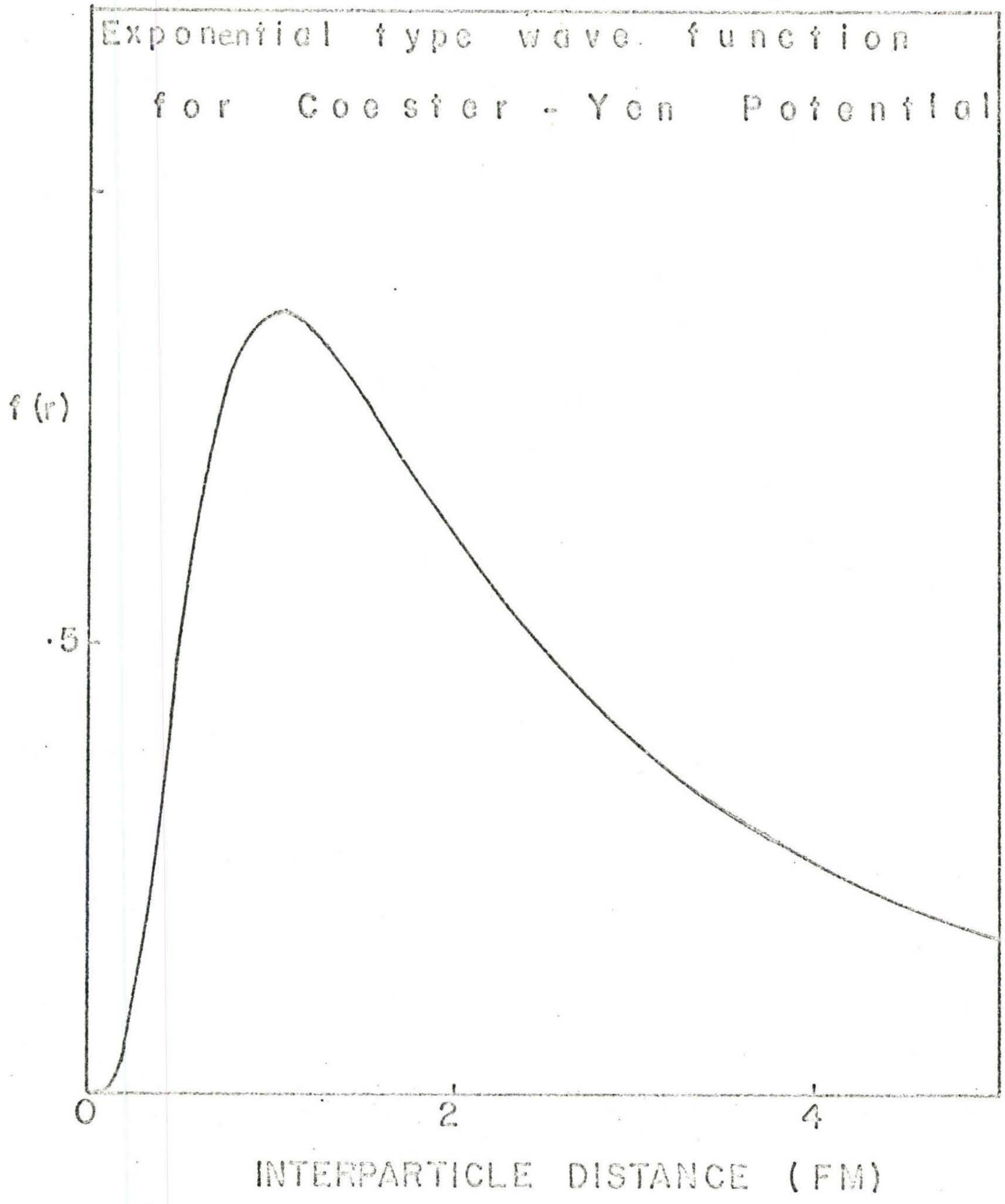
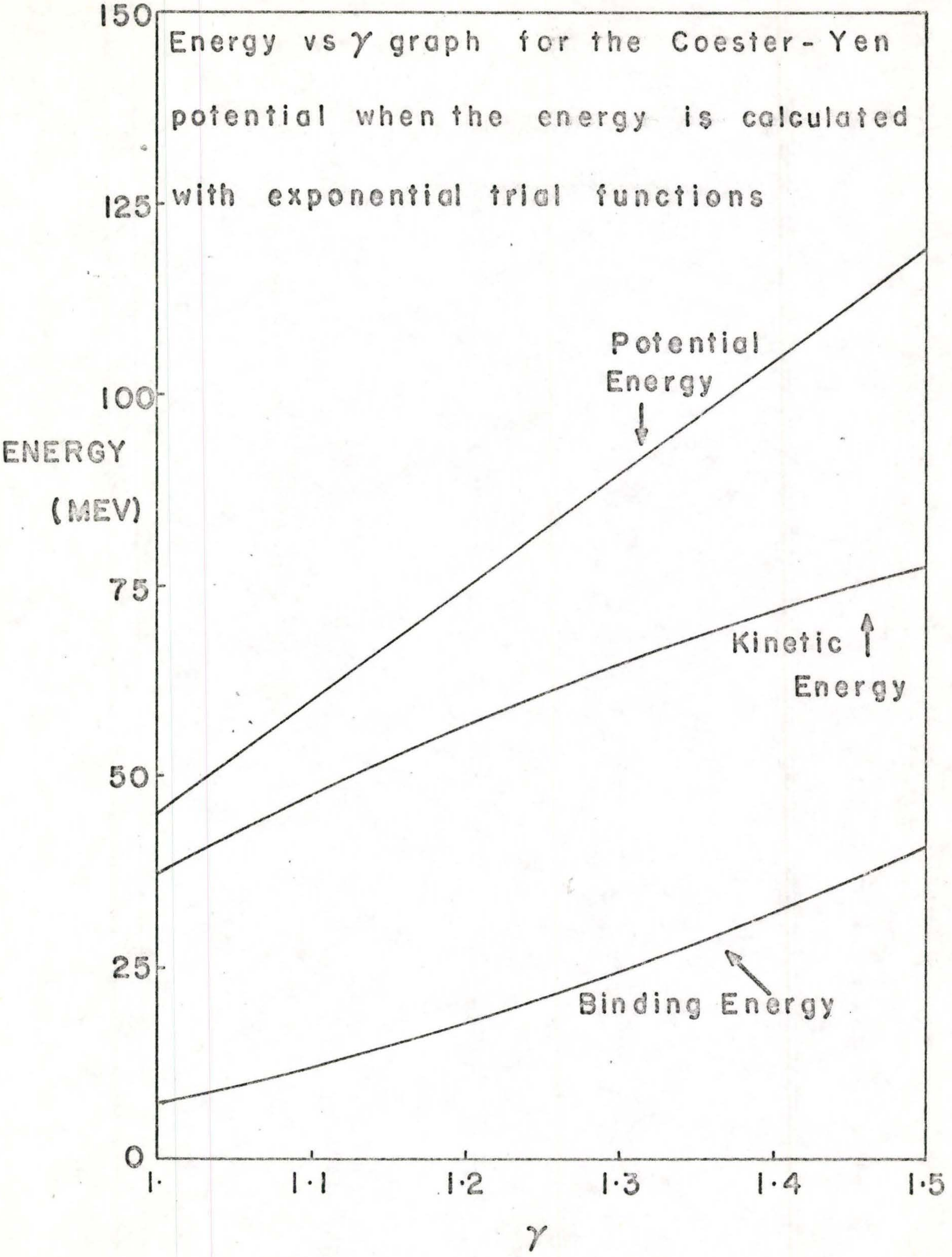

Exponential type wave function
for Coester - Yon Potential
f (r)
.5
0
2
4
INTERPARTICLE DISTANCE (FM)

Figure VI - 6



Energy vs γ graph for the Coester-Yen potential when the energy is calculated with exponential trial functions

Figure VI-7

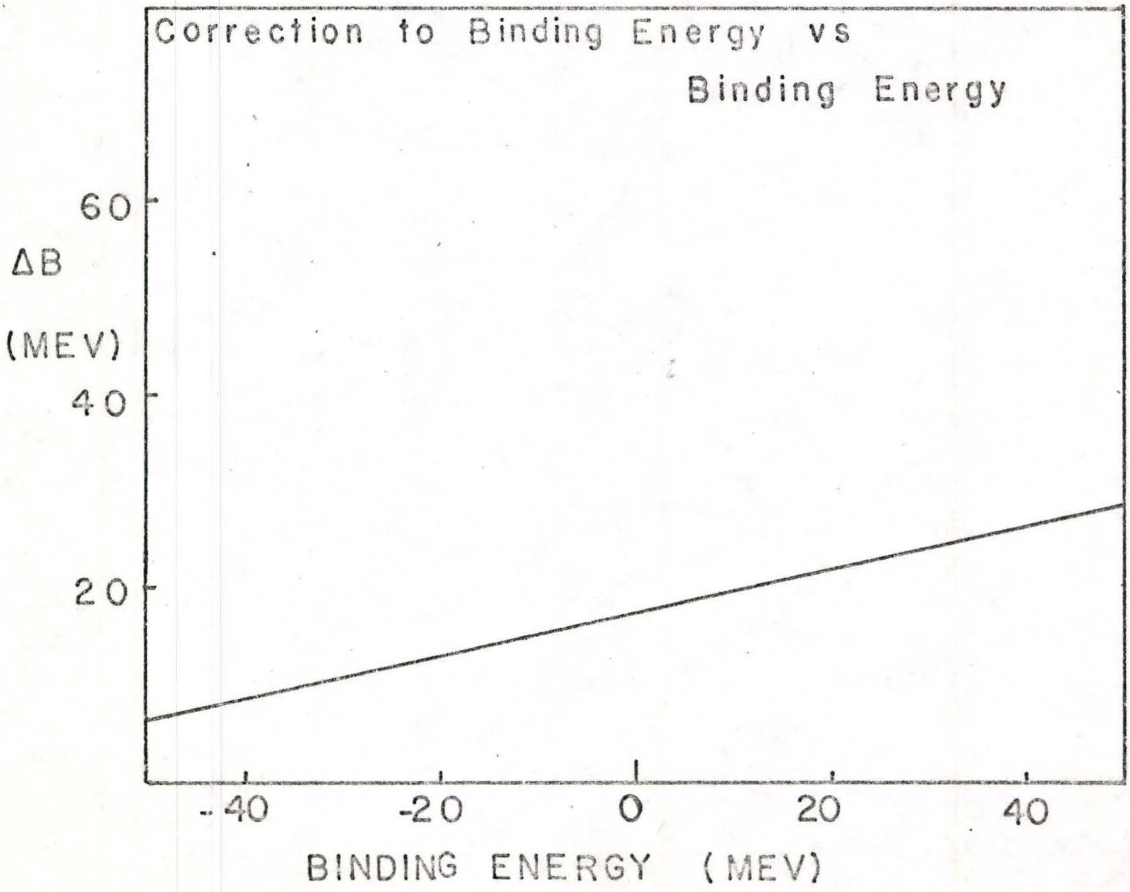

Correction to Binding Energy vs Binding Energy
60
40
20
ΔB
(MEV)
-40
-20
0
20
40
BINDING ENERGY (MEV)

Figure VI-7 is independent of potentials provided that potentials of the same qualitative shape are used, i.e. potentials having a soft repulsive core followed by attraction. The deviation of the Gaussian type wave function from the true wave function gives us the energy correction graph. That the energy correction is due to the behaviour of the wave function rather than the potential can also be seen in the following way.

As we explain later, the functions which have the factor $(\vec{\rho}x\vec{r})^2$ have an unphysical node when $|\vec{r}|$=o, which introduces extra kinetic energy. A large part of the binding energy correction would come from the extraneous kinetic energy. Figure VI-7 is valid then, in the first approximation when Ψ_5 is the dominant state, which is the case for the soft-core potentials. Obviously, the results of the Pease-Feshbach potential should not be corrected using Figure VI-7.

We made a cursory survey of the values of ε which give -7.29 MeV ground state energy. We set δ=o because a small change in the short range behaviour is less likely to have a pronounced effect on the low energy scattering properties of the potential than is a small change in longer range attraction. The values of ε are given in Table VI-8. ε is smallest for states Ψ_1 and Ψ_{10}, i.e. for those states which caused γ to turn negative.

The upshot of our calculation with the Coester-Yen potential is that the potential provides an upper bound to the ground state energy which is close to the experimental energy when an exponential type trial function is used. The Coulomb and mass radii of the system are predicted quite well with this trial function. Soft-cores, like hard-cores, in the potential serve to push out the wave function so that the correct radius is obtained. This simplified model calculation, however, says nothing about the D-state probability in the total wave function.

The calculation with the Gaussian wave function gives no binding at all unless the potential is multiplied by at least 1.2 or unless the core strength is reduced 20%. In both cases, the scattering properties of the potential are altered to the extent that the potential is completely unphysical. If we compare the shapes of the Gaussian type wave function with the shape of exponential type wave function (Figure VI-8 and VI-9) for the Coester-Yen potential multiplied by 1.2, we realize the short-comings of the Gaussian trial functions. The superposition of exponentials (Figure VI-9) is able to suppress the wave function near the origin almost like a wave function produced by a hard core. The Gaussian type functions (Figure VI-8) are non-zero at the origin. They also fall off faster for interparticle distance greater than 2 fm. In brief, the Gaussian trial function is deficient since it picks up too much repulsion of the potential near the origin and too little attraction from the attractive tail of the potential. The magnitudes of these effects may not differ greatly, as we remarked above, for "similar" potentials, e.g. Coester-Yen, Reid, Bressel.

Figure VI-8

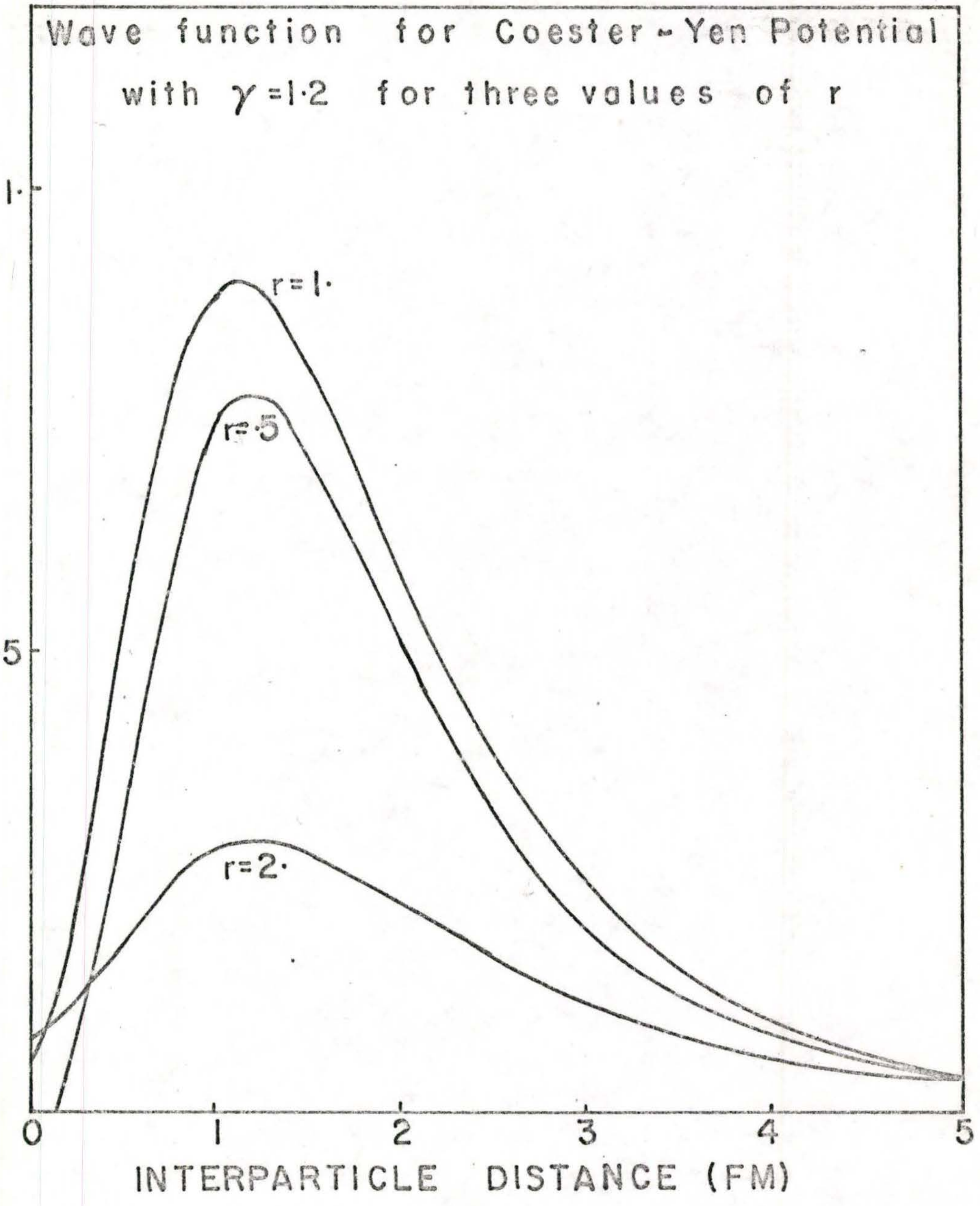

Wave function for Coester-Yen Potential
with γ=1·2 for three values of r
1·
·5
r=1·
r=·5
r=2·
0
1
2
3
4
5
INTERPARTICLE DISTANCE (FM)

Figure VI-9

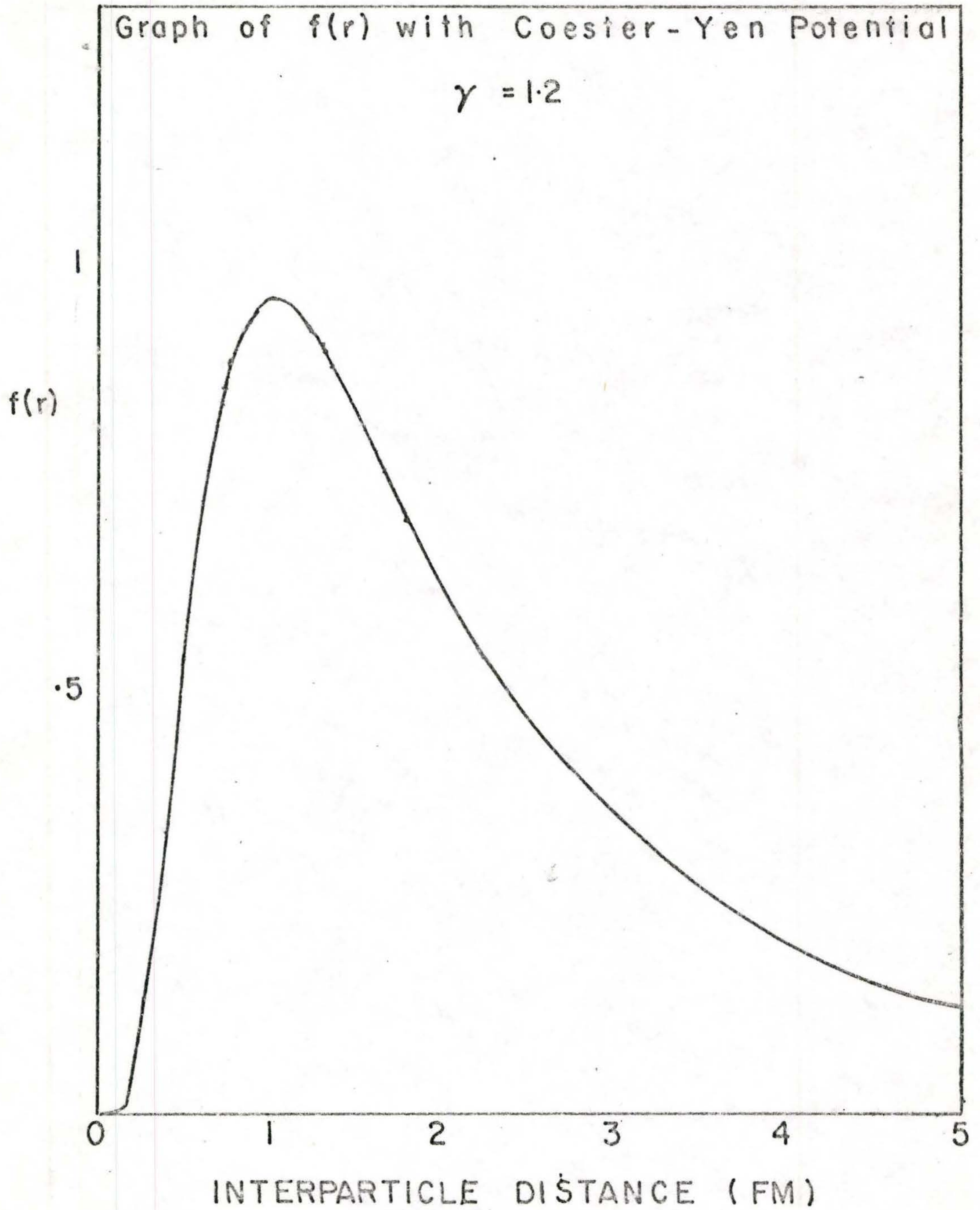

Graph of f(r) with Coester-Yen Potential
γ = 1·2
f(r)
1
·5
0
1
2
3
4
5
INTERPARTICLE DISTANCE (FM)

TABLE VI-5

Minimizing the Force Factor with the Coester-Yen Potential

Force Factor	Energy (MeV)	States
Negative	-8.49	Ψ_1
1.6629	-8.49	Ψ_5
1.4593	-8.49	Ψ_5, Ψ_6
1.5164	-8.49	Ψ_5, Ψ_8
Negative	-8.49	Ψ_{10}

TABLE VI-6

Minimizing the Energy with the Coester-Yen Potential
When the Force Factor=1.6629

Energy	Force Factor	States
-17.00	1.6629	Ψ_1, Ψ_5
-17.02	1.6629	Ψ_5, Ψ_{10}

TABLE VI-7

Minimizing the Energy with Respect to the Linear Parameters with the Coester-Yen Potential Multiplied by 1.4

Non-linear Parameters

State	Parameters			
Ψ_1	.116537	.457265	.921581	7.751768
Ψ_5	.109899	.573794	1.381125	2.320126
Ψ_6	.155427	.821037	1.595433	2.294615
Ψ_8	.145721	1.170600	4.013400	2.446182
Ψ_{10}	.193349	.656363	1.582937	4.722089

Linear Parameters

State	Parameters			
Ψ_1	-.007265	.339133	.067486	-.007583
Ψ_5	.024160	.268653	.177943	.000359
Ψ_6	-.047554	-.712892	-.319796	-.226089
Ψ_8	.007313	.278860	.035842	.160019
Ψ_{10}	.031238	-.065665	-.044404	-.008595

Energy = -10.96 MeV
Kinetic Energy = 71.12 MeV
Potential Energy = -82.08 MeV
$R_{r.m.s.}$ = 1.29 fm.

TABLE VI-7A

Minimizing the Energy with the Coester-Yen Potential Using Exponential Trial Functions

Energy	Kinetic Energy	Potential Energy	Number of Terms	Number of Parameters	Conditions on the Function
-3.728	25.492	-29.220	3	3	$f(o)=f'(o)=o$
-6.718	35.135	-41.849	4	4	$f(o)=f'(o)=f''(o)=o$
-5.286	26.851	-31.137	5	5	$f(o)=f'(o)=f''(o)=f'''(o)=o$
-7.296	37.240	-44.537	5	6	$f(o)=f'(o)=f''(o)=o$

All energies are given in units of MeV.

TABLE VI-8

Minimizing ε with the Coester-Yen Potential (f=o)

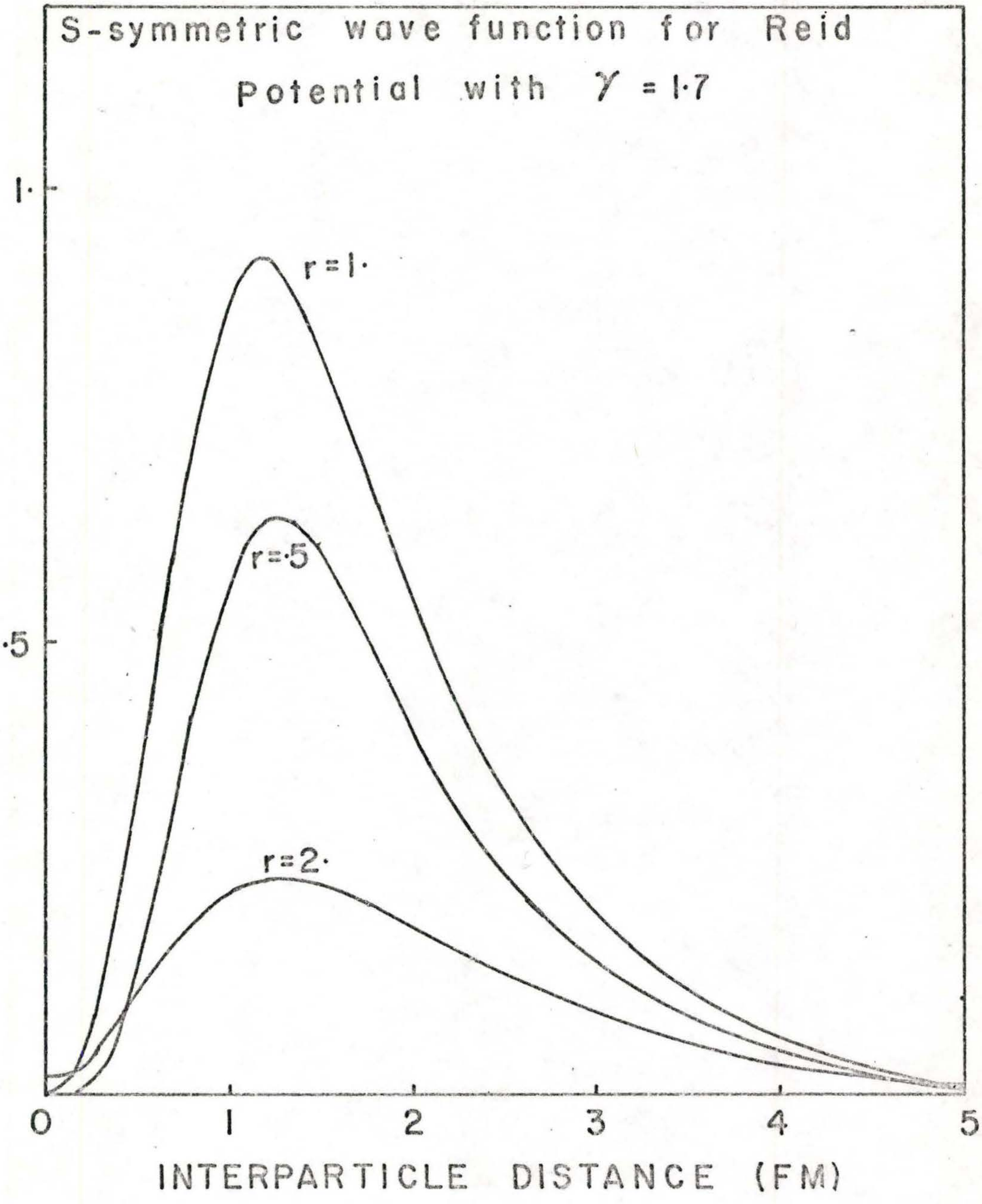
ε	Energy (MeV)	States
.3089	-7.29	Ψ_1
.3986	-7.29	Ψ_5
.7150	-7.29	Ψ_6
.3088	-7.29	Ψ_{10}
.2807	-7.29	Ψ_5, Ψ_6
.3276	-7.29	Ψ_5, Ψ_8
.2217	-7.29	Ψ_5, Ψ_{10}

The Reid Potential

In order to obtain binding with the Reid potential, we have to multiply the potential by γ ($\gamma > 1$), or its repulsive part by $(1-\varepsilon)$ ($o \leqslant \varepsilon < 1$). Ψ_5 is the dominant state. The optimum number of terms in each state is found to be four. We minimize γ to obtain non-linear parameters in each state for which γ remains positive. For the states for which γ turns negative we use the γ found with Ψ_5 as a multiplier of the potential and minimize the energy. With the Reid potential γ is negative when any one of Ψ_1, Ψ_2, Ψ_4, or Ψ_{10} are included. These are the four states which do not tend to zero as ρ approaches zero. We have given a table of results for γ in Table VI-9 and for the energy in Table VI-10. We obtain γ=1.79 for energy equal to 8.5MeV when we use the non-linear parameters in states Ψ_5, Ψ_6, Ψ_7, Ψ_8, Ψ_9 and minimize with respect to the linear parameters only. The final results of the triton properties with the Reid potential multiplied by 1.7 are given in Table VI-11. The angular-averaged wave function of the symmetric S-state is sketched in Figure VI-10. Only a few calculations to obtain ε were done and some of the values are tabulated in Table VI-12, and discussed in the next paragraph.

Our wave functions will not bind the Reid potential at all unless the potential is multiplied by a factor of at least 1.6. The fact that no binding is obtained cannot be attributed to the failure of the trial function to take

Figure VI-10


S-symmetric wave function for Reid
Potential with γ = 1·7
1·
·5
r = 1·
r=·5
r=2·
0
1
2
3
4
5
INTERPARTICLE DISTANCE (FM)

account of the tensor component in the force. If we replace the $^3S_1$ and $^3D_1$ interactions by the ^1S_o and $^1D_2$ interactions and do the calculation for the three-body symmetric S-state, we obtain smaller binding than when we include the three-body D-state and the proper potential. In fact, this result supports our previous conclusion that the symmetric S-state needs the largest improvement. The increase of the overall potential strength will tend to condense the system; the small radius is derived from the large γ, therefore, ε is larger than with the Coester-Yen potential. For the Reid potential, however, we have calculated ε for f=o for the two symmetric S-states, Ψ_1 and Ψ_{10} only, and we know that large part of the binding must be derived from the tensor force interaction between the S- and D-states. In the Coester-Yen potential the tensor contribution to the force is simulated by a stronger central triplet-even force.

The perturbation theory approach in which the change in the repulsive and attractive parts of the potential are both small, does not give a small value for the first order correction to the energy. For instance, if we minimize ε where $\varepsilon=\delta$ for four turns in each of the states Ψ_4, Ψ_5, Ψ_6, Ψ_7, Ψ_{10}, we obtain $\varepsilon=\delta=.098$ for a binding energy of 8.5MeV. The total potential energy, however, is -135.67MeV and the first order correction to the energy is 85.23MeV. Since our calculation does not yield a set of excited states, we cannot find the second order perturbation energy shift. It is clear, however, that the wave function is inadequate to describe this system.

Since it is impossible to obtain binding with the Reid potential except when the potential is multiplied by 1.6 or more, we attempt to apply the correction to the binding energy that must be employed when Gaussian type functions are used. In order to do this we must know what the binding is at $\gamma=1$. In Figure VI-11 we have plotted the binding energy with the Reid potential versus γ. When we extrapolate to $\gamma=1$ we obtain negative binding of -17MeV. Using the correction factor from figure VI-7, we obtain a ground state that is unbound by 4MeV. The final value for the binding is a very crude estimate and should be delimited by the amount ±7MeV. We do feel that this method of extrapolating the curves is valid almost to within the accuracy of the extrapolation because the correction in the binding is mainly due to the Gaussian type wave function that we used. We expect the correction to be independent of the potential since the true wave function, consisting mainly of the symmetric S-state in the case of the Reid potential, would be almost the same shape for both the Coester-Yen and the Reid potential. We have sketched the $^1S_0$ interaction of the Reid potential (Figure VI-12) for comparison with Figure VI-2. In summary, the approximations that were used to obtain the binding are the extrapolation of Figure VI-11 to the binding for $\gamma=1$, the assumption that Figure VI-7 is a straight line and is independent of the potentials used.

Figure VI-II

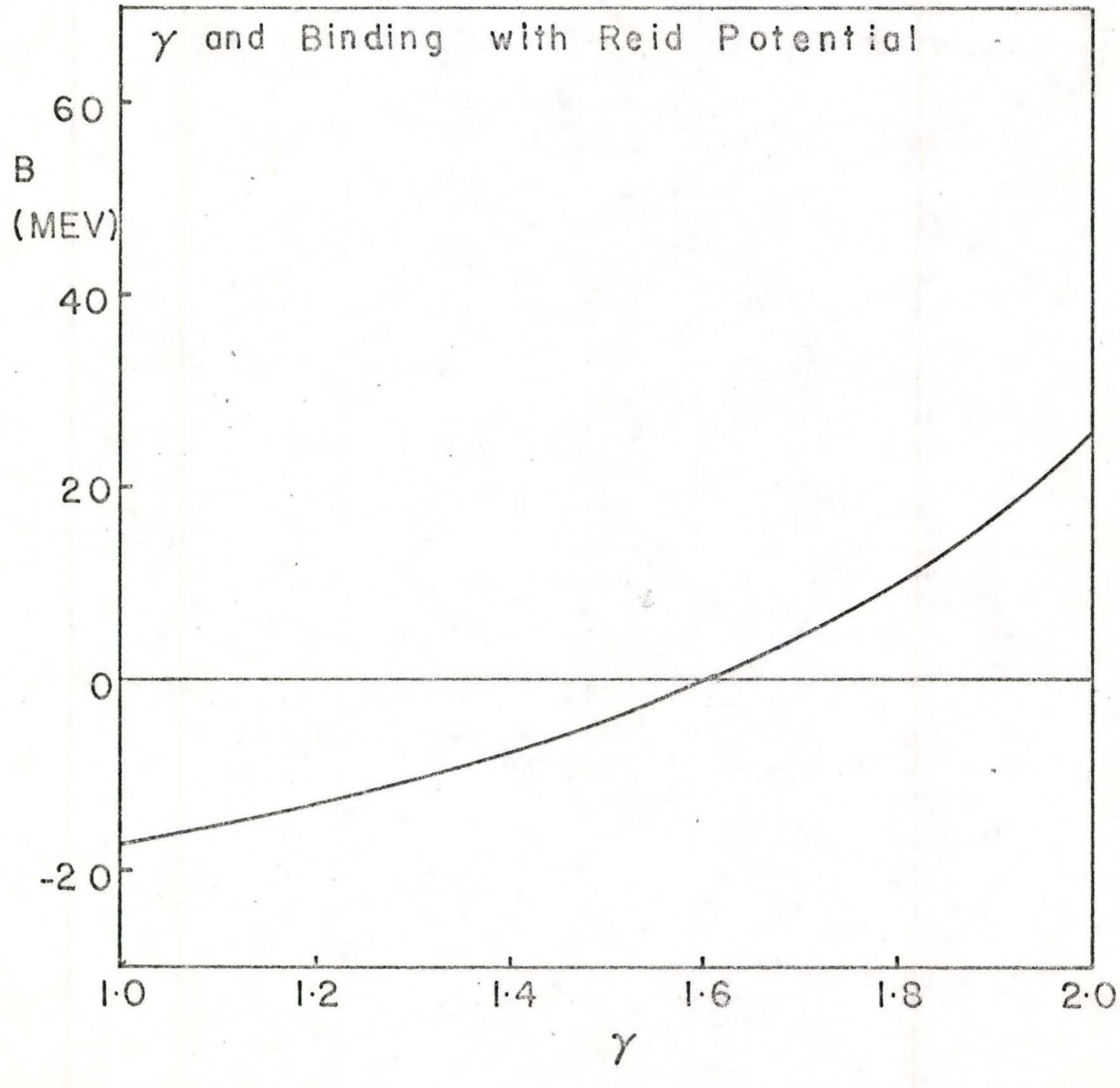

γ and Binding with Reid Potential
B
(MEV)
60
40
20
0
-20
1·0
1·2
1·4
1·6
1·8
2·0
γ

Figure VI - 12

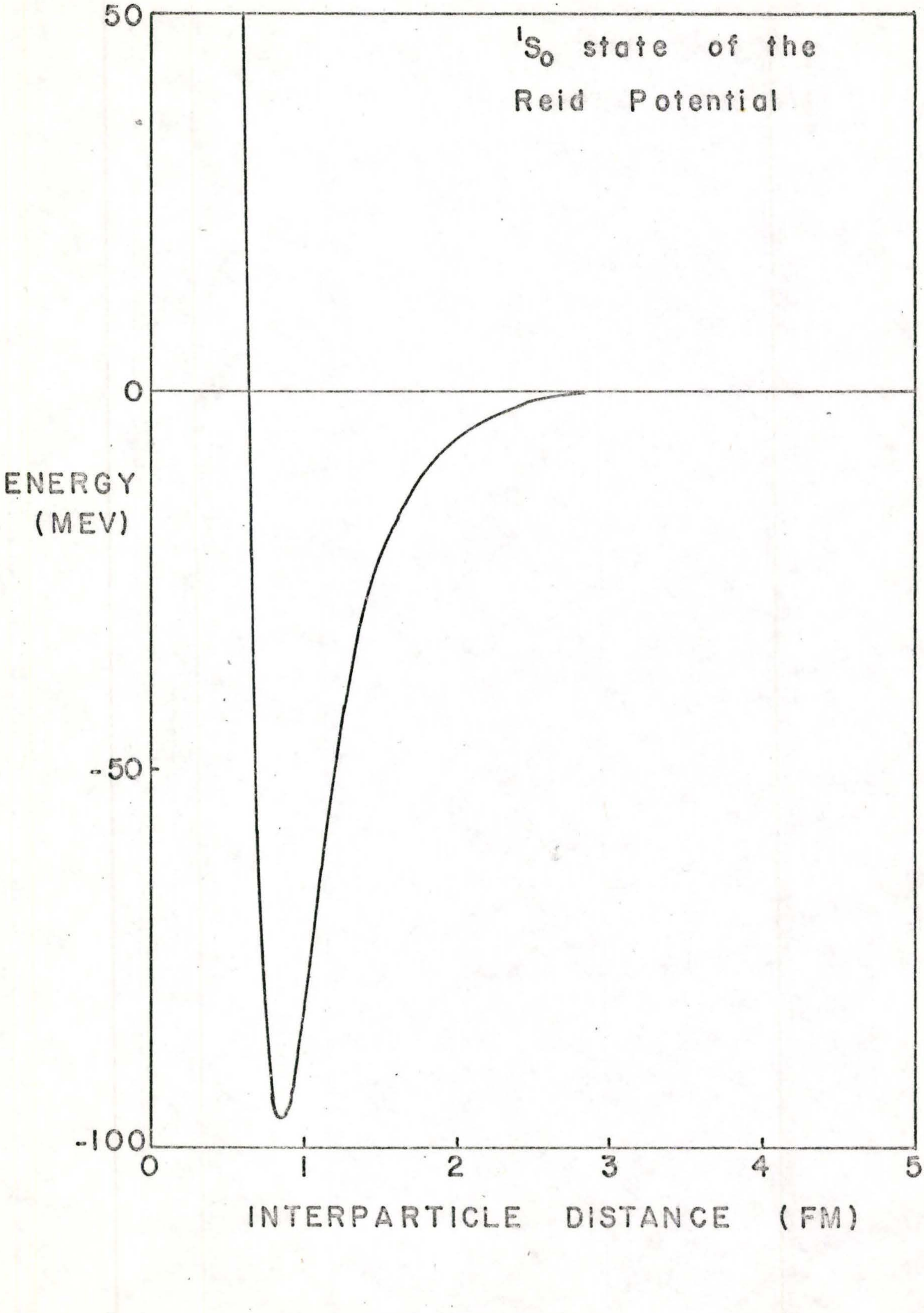

$^1S_0$ state of the Reid Potential
50
0
-50
-100
ENERGY (MEV)
0
1
2
3
4
5
INTERPARTICLE DISTANCE (FM)

TABLE VI-9

Minimizing the Force Factor with the Reid Soft-Core Potential

Force Factor	Energy (MeV)	States
3.577	-8.49	Ψ_5
3.191	-8.49	Ψ_5, Ψ_6
1.951	-8.49	Ψ_5, Ψ_7
3.292	-8.49	Ψ_5, Ψ_8
3.307	-8.49	Ψ_5, Ψ_9
3.577	-8.49	Ψ_5, Ψ_3

TABLE VI-10

Minimizing the Energy with the Reid Soft-Core Potential

Energy (MeV)	Force Factor	States
-10.598	3.577	Ψ_1, Ψ_5
-12.516	3.577	Ψ_2, Ψ_5
-10.565	3.577	Ψ_5, Ψ_{10}

TABLE VI-11

Minimizing the Energy with the Reid Soft-Core Potential Multiplied by 1.7 with Respect to the Linear Parameters Only

Non-linear Parameters

State	Parameters			
Ψ_1	.122266	.920801	.804479	.901478
Ψ_2	.294021	1.404226	.428342	1.839198
Ψ_3	.136587	.868400	.623400	1.200800
Ψ_4	.164765	1.277994	.475161	1.614081
Ψ_5	.108433	.567439	1.371216	3.191201
Ψ_6	.154444	.774191	1.265699	4.073700
Ψ_7	.181700	.724600	1.151000	2.152800
Ψ_8	.136212	.947577	1.500319	5.485319
Ψ_9	.183700	.800000	1.402100	2.060400
Ψ_{10}	.123803	.492203	1.261719	2.792553

Linear Parameters

State	Parameters			
Ψ_1	.006016	.629632	.135078	-.764094
Ψ_2	-.000234	-.000111	-.000164	.000077
Ψ_3	-.000143	-.000492	-.000065	.000539
Ψ_4	-.000191	.000241	-.000283	-.000119
Ψ_5	.001913	.012452	.002673	-.000292
Ψ_6	-.003079	-.030947	-.010784	.002589
Ψ_7	-.000811	-.002499	-.002014	-.003279
Ψ_8	.000173	.010152	.007386	-.001205
Ψ_9	-.000045	-.000075	-.000108	-.000399
Ψ_{10}	-.000711	-.001421	.000468	-.000016

Table VI-11 (Cont'd)

Energy = - 5.06 MeV

Kinetic Energy = 87.28 MeV

Potential Energy = -92.34 MeV

$R_{r.m.s.}$ = 1.36 fm.

P_S = 86.16%

$P_{S'}$ = .47%

P_P = .03%

P_D = 13.35%

TABLE VI-12

Minimizing ε with the Reid Soft-Core Potential

ε	Energy (Mev)	State
.405	-8.49	Ψ_1
.411	-8.49	Ψ_{10}

The Bressel Potential

Since again we could not obtain binding we minimize γ instead of the energy with the Bressel potential. Ψ_5 is the dominant state and four is the optimum number of parameters per state. When the trial function includes states Ψ_2 or Ψ_3, γ is negative. The non-linear parameters are determined by the same procedure that is followed with the Reid potential. The parameters for those states which allowed γ to remain positive are determined by minimizing γ, the others by minimizing the energy while γ is set at the value obtained from the calculation with Ψ_5. The results are given in Tables VI-12 and VI-13. γ is found by minimizing with respect to the linear parameters in states Ψ_1, Ψ_4, Ψ_5, Ψ_6, Ψ_7, Ψ_8, Ψ_9 and its value is $\gamma=1.7013$. Finally, the energy is minimized with respect to the linear parameters using all ten states and $\gamma=1.7$. The results of that calculation are given in Table VI-14. The angular-averaged symmetric S-state wave function is graphed in Figure VI-13. Calculations to find ε with $f=1$ which should simulate the least amount of change in the strengths of the potential indicate that the perturbation approach is very poor since the energy correction is more than half as large as the magnitude of the potential energy.

Figure VI-13

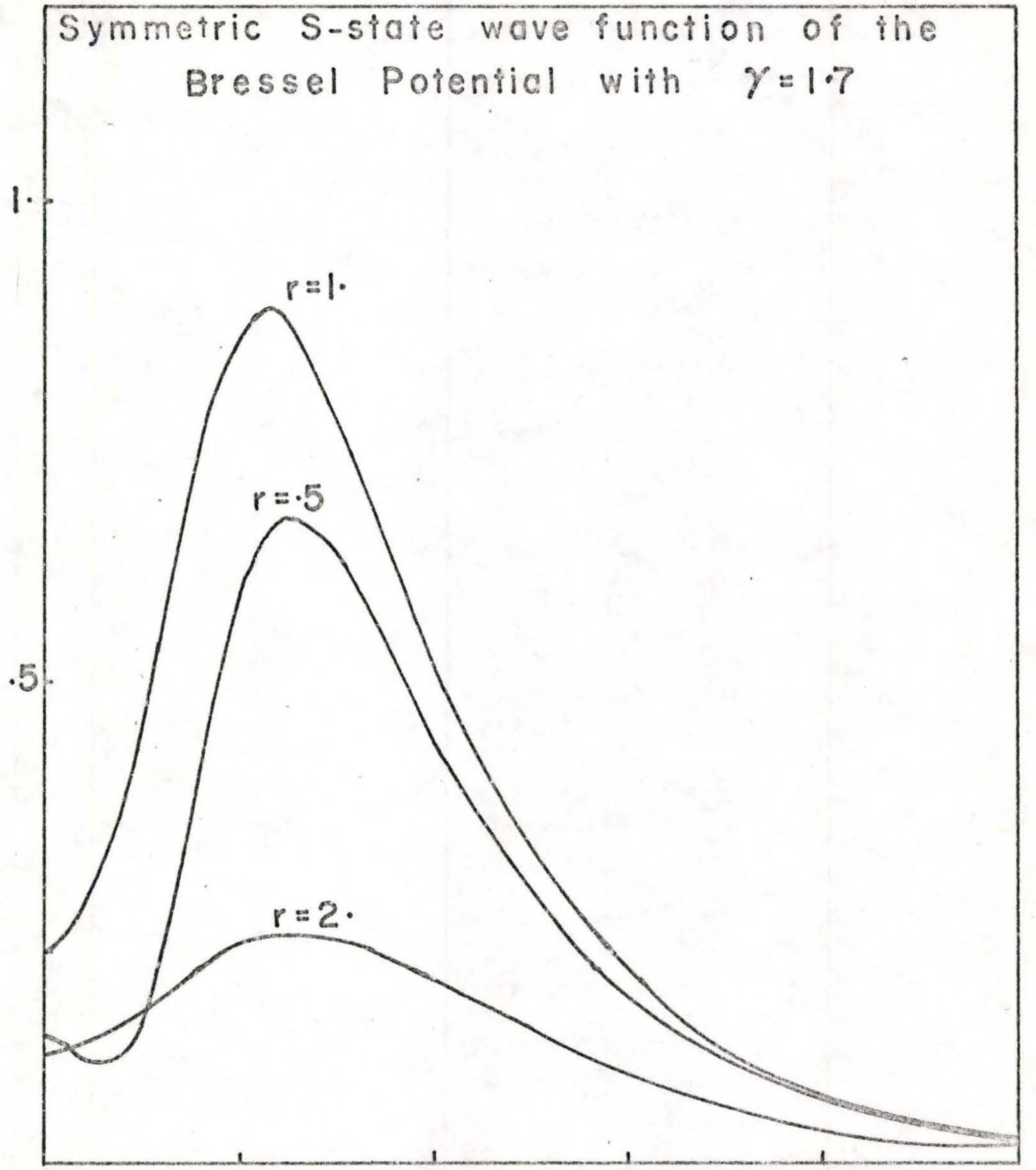

Symmetric S-state wave function of the
Bressel Potential with $\gamma = 1{\cdot}7$
1·
·5
r=1·
r=·5
r=2·
0
1
2
3
4
5
INTERPARTICLE DISTANCE (FM)

TABLE VI-12

Minimizing the Force Factor with the Bressel Potential

Force Factor	Energy (MeV)	States
3.62	-8.49	Ψ_5
3.21	-8.49	Ψ_5, Ψ_6
1.99	-8.49	Ψ_5, Ψ_7
3.31	-8.49	Ψ_5, Ψ_8
3.48	-8.49	Ψ_5, Ψ_9
3.18	-8.49	Ψ_5, Ψ_{10}
3.18	-8.49	Ψ_1, Ψ_5
2.49	-8.49	Ψ_4, Ψ_5

TABLE VI-13

Minimizing the Energy with the Bressel Potential When γ=3.623

Energy (MeV)	Force Factor	States
-10.25	3.623	Ψ_2, Ψ_5
- 8.49	3.623	Ψ_3, Ψ_5

TABLE VI-14

Minimization of the Energy with Respect to the Linear Parameters with the Bressel Potential When $\gamma=1.7$

Non-linear Parameters

State	Parameters			
Ψ_1	.137500	.368750	.881250	1.762500
Ψ_2	.141688	.422130	1.947900	1.890200
Ψ_3	.088429	.436149	.967798	1.460887
Ψ_4	.105625	.401562	1.092187	2.240625
Ψ_5	.257390	.671836	1.556250	4.730625
Ψ_6	.103227	.655229	1.111927	3.931375
Ψ_7	.266875	.808537	1.631200	2.47500
Ψ_8	.165844	.988212	1.427300	2.320312
Ψ_9	.198250	.539025	1.304960	2.475000
Ψ_{10}	.127211	.441068	1.489678	6.015927

Linear Parameters

State	Parameters			
Ψ_1	.3773417	-.271386	.523136	-.140175
Ψ_2	-.011329	-.010251	-.032250	.035490
Ψ_3	-.004006	-.013622	-.001180	.001883
Ψ_4	-.006913	-.035139	.009339	.000177
Ψ_5	.036282	.316735	.053569	-.006797
Ψ_6	.017566	-.211542	-.525767	.054505
Ψ_7	-.041484	-.109102	-.105997	-.078428
Ψ_8	-.002070	.033903	.137185	.007535
Ψ_9	.008023	-.001633	-.020704	-.007317
Ψ_{10}	-.010716	.041845	-.063696	-.002685

Table VI-14 (Cont'd)

Energy = $-$ 8.98 MeV
Kinetic Energy = 69.34 MeV
Potential Energy = -78.32 MeV
$R_{r.m.s.}$ = 1.38 fm.

P_S = 86.81%
$P_{S'}$ = .36%
P_P = .04%
P_D = 12.79%

Comparison of the Trial Functions

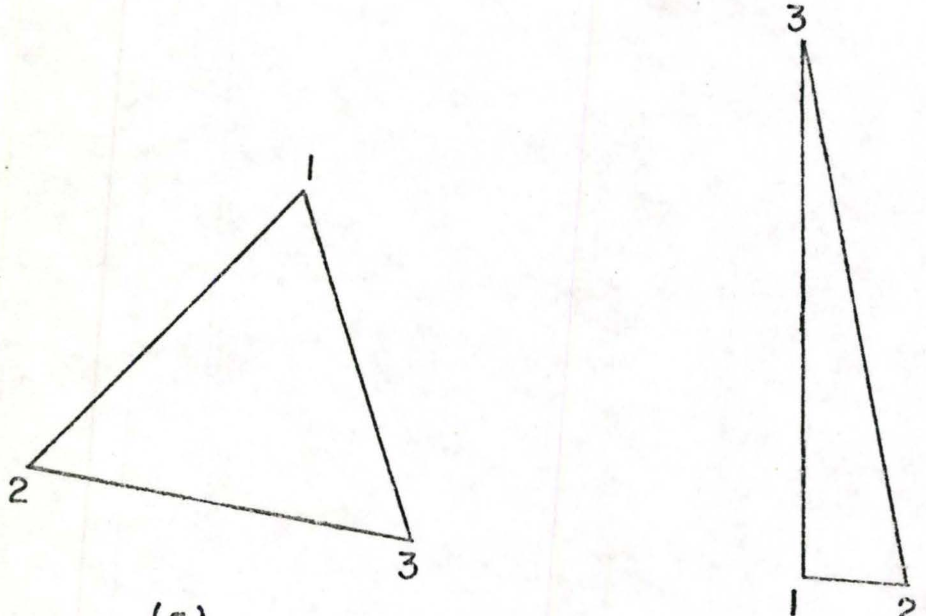
We have found that the Gaussian type of trial function will bind the triton with the Pease-Feshbach potential but not with any potential that has a soft repulsive core. The exponential function will bind the triton with the Pease-Feshbach potential (PF52) and bind it with greater binding energy than we were able to obtain. A superposition of exponentials will also bind the Coester-Yen potential which has a soft repulsive core. There are two features of the trial function that need to be examined closely. The first is the exponential or Gaussian decay and the other is the correlations that are built in the trial function. Whether there is a tensor component present in the potential or not, does not seem to have much bearing on the type of trial function that we use. It is true that a smaller force factor was found with the Coester-Yen than with either of the other two soft-core potentials, but the tensor force gives approximately the same D-state probabilities with both the exponential and Gaussian trial functions when applied to the Pease-Feshbach potential. The large D-state probability with both the Bressel and the Reid potential are due to the condensed system (γ=1.7) and the inadequacy of the symmetric S-state component of the trial function. Our discussion will by and large be limited to the symmetric S-state whose probability should be approximately 95% of the total wave function.

In order to note the difference between the fall offof the superposition of exponentials and Gaussians at large interparticle distance, we should compare Figures VI-8 and VI-9. From them it is evident that the exponential function decays slower than the superposition of Gaussians at any of the positions of the third particle that are indicated. This behaviour prevents the Gaussian type trial function from picking up a large portion of the attraction that can be derived from the potential for distances greater than 1.5 fm. The inclusion of some long-range terms in the superposition of Gaussians, that we had hoped for, did not materialize. The peak of the Gaussian type function is shifted slightly to the longer range part of the graph when compared to the peak of the exponential function. If we compare the location of the peaks to the location of the minimum of the Coester-Yen potential, we see that the exponential peak is closer to the minimum of the potential than is the peak of the Gaussian type functions. In short, the superposition of exponentials gives a better shape than does the superposition of any arbitrary number of Gaussians of the types that we have used.

The comparison between superposition of exponentials and sums of Gaussians is not altogether valid without some qualifications, although the features that we mentioned certainly do indicate what the shortcomings of the Gaussians are. The fact is, however, that the exponential type functions are defined such that the position of the third particle does not influence the two particle correlation at all. For the Gaussian type wave function the peak of the wave function occurs at different places for different values of r (see Figures VI-10, and VI-13). The shift in maxima is less than .25 fm, but within a small distance of this magnitude the potential strength may change by as much as 30MeV (see Figures VI-2 and VI-12).

The source of this kind of correlation is that the argument of the exponential in our Gaussian type functions is (ρ^2+r^2). This means that as far as the decay of the function is concerned, for a particular (ρ^2+r^2) no distinction is made between the configuration of three particles where the distance between particles 1 and 2 is small and the third particle a large distance removed from these two (Figure VI-14(b)) and the situation which has almost equal interparticle distances (Figure VI-14(a)). This argument is especially valid in the case of the Pease-Feshbach potential since Ψ_1 is dominant state with it. The same situation arises when one does a Feshbach-Rubinow calculation (FR55) which calculates the best wave function dependent on a single coordinate, $R = 1/2(r_{12} + r_{23} + r_{13})$. Such a wave function does also not distinguish between the two con-

Figure VI-14



(a)

(b)

figurations shown in Figure VI-14. It is not surprising therefore that neither the spin-averaged Coester-Yen potential nor the ^1S_o-state interaction of the Reid potential gives binding in a Feshbach-Rubinow calculation.

In order to ensure that our trial function contained terms which vanish as the interparticle distance tends to zero, we multiplied Ψ_1 by ρ^{2n}, n=1,2, or 3. If we then expand the wave function in powers of ρ those terms have as first term in the expansion ρ^{2n}. When n=1, the wave function varies as ρ^2 for small interparticle distances. The exponential type wave function we used with the condition that $f(o) = f'(o) = f''(o) = o$ varies as $\rho^{5/2}$ for small ρ. Although the power of ρ is not exactly the same in both cases, they are close enough so that both functions have the same qualitative behaviour at small interparticle distance. Because of the symmetry requirement, however, we were forced to use this multiplier in conjunction with r^{2n} since we had to multiply Ψ_1 by $(\vec{\rho}x\vec{r})^{2n}$. This introduces an unphysical constraint on the wave function. When the three particles lie almost on a straight line, r tends to zero and hence the amplitude of the wave function vanishes. When the interparticle distances $r_{13}=r_{12}=1$ fm and interparticle distance $r_{12} \simeq 2$ fm, there is no physical reason why the wave function should vanish. The feature that gives us more desirable behaviour of the trial function at small interparticle distance has the side-effect of introducing an extra node in the wave function with corresponding greater overall kinetic energy.

The different behaviour of the wave function when used in conjunction with a Yukawa-shaped barrier or with a square barrier as found in the Bressel potential is shown in Figures VI-10 and VI-13. With the Bressel potential the wave function is not so adverse to having a finite amplitude at zero interparticle distance as with the Yukawa type barrier found in the Reid potential. This is due to the singularity of Reid's potential at the origin; the Bressel potential has strong but finite repulsion throughout the repulsive force region. For the same reason Ψ_1 has greater probability in Bressel's than in Reid's wave function, and consequently the kinetic energy is less for the Bressel than for the Reid potential. The wave function has a somewhat different behaviour for different shapes of the soft cores and comparison of results obtained for the two different potentials should be made with reservation.

The Binding Energy in Triton Found with the Various Potentials

One can make several observations about the potentials that we have used in the triton binding energy calculation. The statements about the binding of the triton with the Reid or the Bressel potential, however, cannot be as definitive as we would like because of the deficiencies of the trial function.

The Coester-Yen potential binds the triton with almost the experimental binding energy. Since we do a variational calculation we obtain an upper bound to the experimental ground state energy and hence the discrepancy between theoretical and experimental binding may be reduced by the choice of a trial function more elaborate than the sum of exponentials that we used. Although the potential is very simplistic and one should not expect very accurate results from it, the calculated radii agree with the experimentally determined Coulomb and mass radii.

The calculations with the Reid potential indicate that with the type of trial functions we used we cannot obtain binding of the triton. When we introduce the correction in binding that is necessary since we used Gaussian type trial functions, we obtain binding of -4 ± 7MeV. This is a very rough estimate and we cannot compare our results with the accurate results of Blatt et al. (BD67) and Davies (D67). We can say, however, that the upper bound of the triton ground state energy calculated with the Reid potential is not so low that the softcore increases the binding to the extent that the Reid potential would give unreasonable results in the triton. In fact, it appears that if a more accurate calculation were done, i.e. with the accuracy of Blatt *et al*., the Reid potential would give binding energy of the triton of the order of magnitude that Blatt *et al*. obtained with the hard-core potentials. It is premature at this stage to say whether the Reid soft-core would give an increased binding over the hard-core potentials.

Not much more can be said of the Bressel potential than of the Reid potential except that the Bressel potential gives slightly more binding energy than the Reid potential. Since the Hamada-Johnston potential binds the triton with at least 5.7MeV binding (D67) and the Bressel potential is derived from the Hamada-Johnston one would expect somewhat higher binding with the Bressel than with the Hamada-Johnston. In order to determine this conclusively a calculation like that of Blatt *et al*. should be done with the Bressel potential, albeit with built in short-range correlation to take account of the soft core. For the Reid potential one would need to find a manageable way of projecting two-body LSJ states from exponential type wave functions and then proceed with the calculation.

CHAPTER VII

SUMMARY AND CONCLUSION

We have studied the triton variational problem with two types of trial function and four potentials. The superposition of Gaussians as a trial function is ideally suited for projecting out the two-body LSJ dependence from the three-body trial function. Employing the Cohen and Willis classification (CW62) of three-body states, we have succeeded in writing the three-body wave function as a sum of terms each of which has definite two-body LSJ dependence. The sum of exponentials as a trial function is known to give good results (VK67). The superposition of Gaussians, however, do not give as good a result of the triton binding energy as does a superposition of exponential trial functions. The correction that must be applied to the binding when it has been determined by means of the Gaussian type trial function is given in Figure VI-7 for potentials with strong repulsive cores. For potentials without a repulsive core, the Gaussian type wave function gives underbinding although not so seriously as with the soft-core potentials. With the Pease-Feshbach potential the Gaussian type trial function gives about

4 to 5 MeV too little binding.

The Coester-Yen potential, although it is a central spin-dependent Serber potential, gives very good results in the triton, binding it with 7.3MeV and giving a mass radius of 1.7 fm. Our analysis shows that the Reid potential does not overbind the triton. If it did, this potential would have to be rejected for other nuclear structure calculations. Since the Bressel potential gives only slightly more binding than the Reid potential, it is thought not to overbind the triton either. No definitive values for the binding with the last two potentials can be quoted until different methods have been developed.

APPENDIX A

SIX-DIMENSIONAL HARMONIC OSCILLATOR FUNCTIONS AS A BASIS FOR TRIAL FUNCTIONS IN THE TRITON

If we use the vectors which have been defined in Chapter II, we can write the Hamiltonian for the six-dimensional harmonic oscillator in terms of these vectors. The Hamiltonian is

$$H_o \equiv -\frac{1}{2}(\nabla_\rho{}^2 + \nabla_r{}^2) + 2\lambda^2(\rho^2 + r^2) \tag{1}$$

This Hamiltonian has a set of eigenstates and eigenvalues which are the solution of the equation

$$H_o\,\psi_n = E_n\psi_n \tag{2}$$

The ground state is $\psi_o = \left(\frac{2\lambda}{\pi}\right)^{3/2} e^{-\lambda(\rho^2+r^2)}$. This is a typical term of the expansion in Ψ_1. The ground state energy is $E_o = 6\lambda$. We now define the creation and annihilation operators (see D65 for a more formal treatment)

$$\vec{A}^+ = \frac{1}{\sqrt{\lambda}}(2\lambda\vec{\rho} - \vec{\nabla}_\rho) \qquad \vec{A} = \frac{1}{\sqrt{\lambda}}(2\lambda\vec{\rho} + \vec{\nabla}_\rho)$$
$$\vec{B}^+ = \frac{1}{\sqrt{\lambda}}(2\lambda\vec{r} - \vec{\nabla}_r) \qquad \vec{B} = \frac{1}{\sqrt{\lambda}}(2\lambda\vec{r} + \vec{\nabla}_r) \tag{3}$$

We can show that the commutators $[A_i, A_j{}^+]=[B_i, B_j{}^+] = \delta_{ij}$. All other commutators are zero. The Hamiltonian can be written in terms of these operators:

$$H_o = 6\lambda + 2\lambda(\vec{A}^{+}\cdot\vec{A} + \vec{B}^{+}\cdot\vec{B}) \tag{4}$$

and $$[H_o, \vec{A}^{+}] = 2\lambda\vec{A}^{+} \;,\; [H_o, \vec{B}^{+}] = 2\lambda\vec{B}^{+} \tag{5}$$

The excitation per mode of excitation is 2λ as is indicated by the expressions:

$$\begin{aligned} H_o(\vec{A}^{+}\,\psi_n) &= (E_n + 2\lambda)\;A^{+}\psi_n \\ H_o(\vec{B}^{+}\,\psi_n) &= (E_n + 2\lambda)\;B^{+}\psi_n \end{aligned} \tag{6}$$

$\vec{A}^{+}$ and $\vec{B}^{+}$ have the same permutation symmetry as the vectors $\vec{\rho}$ and $\vec{r}$. We can therefore form operators from $\vec{A}^{+}$ and $\vec{B}^{+}$ with definite symmetry. The three lowest order symmetric operators are 1, $(\vec{A}^{+})^2 + (\vec{B}^{+})^2$, $(\vec{A}^{+} \times \vec{B}^{+})^2$.

$$\psi_2 = [(\vec{A}^{+})^2 + (\vec{B}^{+})^{2}]\psi_o = [-6 + 2\lambda(\rho^2 + r^2)]\psi_o \tag{7}$$

$$\psi_4 = [\vec{A}^{+} \times \vec{B}^{+}]^2\psi_o = [16\lambda^2(\vec{\rho} \times \vec{r})^2 - 8\lambda(\rho^2 + r^2) + 6]\psi_o \tag{8}$$

Thus we can write according to our notation for states in Chapter III:

$$\Psi_{10} = (\rho^2 + r^2)\psi_o = \frac{1}{2\lambda}\,\psi_2 + \frac{3}{\lambda}\,\psi_o \tag{9}$$

$$\Psi_5 = (\vec{\rho} \times \vec{r})^2\psi_o = \frac{1}{16\lambda^2}\,\psi_4 + \frac{1}{4\lambda^2}\,\psi_2 + \frac{9}{8\lambda^2}\,\psi_o \tag{10}$$

The states Ψ_1, Ψ_5, Ψ_{10} are therefore linear combinations of the three lowest energy states which are base functions of the symmetric representation and are eigenstates of the six-dimensional harmonic oscillator.

APPENDIX B

VARIATIONAL CALCULATION OF THE TRITON USING A SUPERPOSITION OF EXPONENTIAL FUNCTIONS AS THE TRIAL FUNCTION

The three interparticle distances are denoted by a, b, and c. Ψ is an S-state wave function. All S-states may be written as functions of ρ^2, r^2, and $(\vec{\rho}\cdot\vec{r})$ only. The kinetic energy operator is $-\frac{\hbar^2}{2M}K$ where M is the nucleon mass. For all states

$$K = \nabla_r^{\,2} + \nabla_\rho^{\,2} \tag{1}$$

If we assume Ψ is an S-state function dependent on ρ^2, r^2, and $(\vec{\rho}\cdot\vec{r})$ only we can write K in terms of interparticle distances, i.e.

$$K = 2\{ \frac{d^2}{da^2} + \frac{d^2}{db^2} + \frac{d^2}{dc^2} + \frac{2}{a}\frac{d}{da} + \frac{2}{b}\frac{d}{db} + \frac{2}{c}\frac{d}{dc} + \frac{a^2+b^2-c^2}{2ab}\frac{d^2}{dadb} + \frac{b^2+c^2-a^2}{2bc}\frac{d^2}{dbdc} + \frac{c^2+a^2-b^2}{2ca}\frac{d^2}{dcda} \} \tag{2}$$

The expectation value of the kinetic energy is proportional to

$$\langle\Psi|K|\Psi\rangle = 2\int_0^\infty da \int_0^\infty db \int_{|a-b|}^{(a+b)} dc\ \Psi\{ \frac{d^2\Psi}{da^2} + \frac{d^2\Psi}{db^2} + \frac{d^2\Psi}{dc^2}$$

$$+ \frac{2}{a}\frac{d\Psi}{da} + \frac{2}{b}\frac{d\Psi}{db} + \frac{2}{c}\frac{d\Psi}{dc} + \frac{b^2+c^2-a^2}{2bc}\,\frac{d^2\Psi}{dbdc}$$

$$+ \frac{a^2+b^2-c^2}{2ab}\,\frac{d^2\Psi}{dadb} + \frac{c^2+a^2-b^2}{2ac}\,\frac{d^2\Psi}{dadc} \Big\}\, abc \qquad (3)$$

By the use of Gauss's theorem (W61, p.235) equation (3) can be rewritten in the form

$$<\Psi|K|\Psi> \;=\; 2\int_0^\infty da \int_0^\infty db \int_{|a-b|}^{(a+b)} dc \;\Big\{ -\left(\frac{d\Psi}{da}\right)^2 - \left(\frac{d\Psi}{db}\right)^2 - \left(\frac{d\Psi}{dc}\right)^2$$

$$- \frac{b^2+c^2-a^2}{2bc}\left(\frac{d\Psi}{db}\right)\left(\frac{d\Psi}{dc}\right)$$

$$- \frac{a^2+b^2-c^2}{2ab}\left(\frac{d\Psi}{da}\right)\left(\frac{d\Psi}{db}\right)$$

$$- \frac{c^2+a^2-b^2}{2ac}\left(\frac{d\Psi}{da}\right)\left(\frac{d\Psi}{dc}\right)\Big\}\, abc \qquad (4)$$

If we assume that $\Psi(a,b,c)$ is separable in the three variables, i.e. $\Psi(a,b,c) = f(a)\, g(b)\, h(c)$, then $\left(\frac{d\Psi}{db}\right)\left(\frac{d\Psi}{dc}\right) = \Psi\,\frac{d^2\Psi}{dbdc}$. Adding equation (1) and (2) and dividing the sum by 2, we obtain

$$<\Psi|K|\Psi> \;=\; \int_0^\infty da \int_0^\infty db \int_{|a-b|}^{(a+b)} dc \;\Big\{ \Psi\,\frac{d^2\Psi}{da^2} + \Psi\,\frac{d^2\Psi}{db^2}$$

$$+ \Psi\,\frac{d^2\Psi}{dc^2} + \frac{2}{a}\,\Psi\,\frac{d\Psi}{da} + \frac{2}{b}\,\Psi\,\frac{d\Psi}{db} + \frac{2}{c}\,\Psi\,\frac{d\Psi}{dc}$$

$$- \left(\frac{d\Psi}{da}\right)^2 - \left(\frac{d\Psi}{db}\right)^2 - \left(\frac{d\Psi}{dc}\right)^2 \Big\}\, abc \qquad (5)$$

Because of the symmetry of the three variables, expression (5) can be written in the simple form

$$<\Psi|K|\Psi> = 3 \int_0^\infty da \int_0^\infty db \int_{|a-b|}^{(a+b)} dc \;\{\Psi \frac{d^2\Psi}{da^2} + \frac{2}{a} \Psi \frac{d\Psi}{da} - \left(\frac{d\Psi}{da}\right)^2 \}\; abc \qquad (6)$$

Actually there is a factor of $\frac{8\pi^2}{3\sqrt{3}}$ in front of the integrals from the angular integration that was done in order to obtain (3). This factor, however, cancels with a similar factor appearing in the normalization integral.

Now we invoke the assumption that $\Psi(a,b,c)$ is symmetric under interchange of particles, i.e. $\Psi(a,b,c) = f(a)\, f(b)\, f(c)$.

$$<\Psi|K|\Psi> = \int_0^\infty \{a\, f(a)\, f''(a) - a[f'(a)]^2 + 2\, f(a)f'(a)\}F(a)da \qquad (7)$$

where

$$F(a) = \int_0^\infty db \int_{|a-b|}^{(a+b)} dc\; \{b[f(b)]^2\}\{c[f(c)]^2\} \qquad (8)$$

The particular form that we chose for f(a) for the variational calculation is

$$f(a) = a^{-1/2} \sum_{i=o}^{k} c_i\, e^{-\lambda_i a} \qquad (9)$$

with $\sum_{i=o}^{k} c_i = o$ so that $f(o) = o$. (10)

The c_i's that are not yet determined by the normalization and condition (10) and the λ_i's are the variational parameters. F(a) can be evaluated explicitly with the form of f(a) that we have chosen.

$$F(a) = \sum_{\substack{i,j,m,n=o \\ \lambda_i+\lambda_j-\lambda_m-\lambda_n \neq o}}^{k} \frac{-4c_i c_j c_m c_n}{(\lambda_i+\lambda_j+\lambda_m+\lambda_n)(\lambda_i+\lambda_j-\lambda_m-\lambda_n)} e^{-(\lambda_i+\lambda_j)a}$$

$$+ \sum_{\substack{i,j,m,n=o \\ \lambda_i+\lambda_j-\lambda_m-\lambda_n \neq o}}^{k} \frac{c_i c_j c_m c_n}{\lambda_i+\lambda_j} \; a \; e^{-(\lambda_i+\lambda_j)a} \tag{11}$$

The normalization integral is

$$N = \int_o^\infty \{ a[f(a)]^2 \} F(a) da$$

$$N = \sum_{\ell,p=o}^{k} c_\ell c_p \{ \sum_{\substack{i,j,m,n=o \\ \lambda_i+\lambda_j-\lambda_m-\lambda_n \neq o}}^{k} \frac{-4c_i c_j c_m c_n}{(\lambda_i+\lambda_j+\lambda_\ell+\lambda_p)(\lambda_i+\lambda_j-\lambda_m-\lambda_n)(\lambda_i+\lambda_j+\lambda_m+\lambda_n)}$$

$$+ \sum_{\substack{i,j,m,n=o \\ \lambda_i+\lambda_j-\lambda_m-\lambda_n = o}}^{k} \frac{c_i c_j c_m c_n}{(\lambda_i+\lambda_j)(\lambda_i+\lambda_j+\lambda_\ell+\lambda_p)^2} \} \tag{12}$$

The kinetic energy is

$$-\frac{\hbar^2}{2M} <\Psi|K|\Psi> \;=\; 3\int_0^\infty \sum_{i,j=o}^{k} c_i c_j \{20.735\; [\;\frac{1}{2}\, a^{-2}$$

$$+ \frac{1}{2}\, a^{-1}\; (\lambda_i+3\lambda_j)$$

$$- \lambda_j^{\,2} + \lambda_i\lambda_j]\}\; e^{-(\lambda_i+\lambda_j)a}\; F(a)da \qquad (13)$$

The potential energy is

$$<\Psi|V|\Psi> \;=\; 3\int_0^\infty \sum_{i,j=o}^{k} c_i c_j\; e^{-(\lambda_i+\lambda_j)a}\; V(a)\; F(a)da \qquad (14)$$

The expectation value of the energy is given by

$$E = \frac{1}{N}\,\{-\,\frac{\hbar^2}{2M}\, <\Psi|K|\Psi> \;+\; <\Psi|V|\Psi>\} \qquad (15)$$

Because of the condition $\sum_{i=o}^{k} c_i = o$, the integrands are zero at the origin for the kinetic energy and for potentials of exponential or Yukawa shape. The parameters λ_i and c_i are varied until a minimum in the energy is found. One can include as many terms as one feels are necessary due to the complex behaviour of the potential, or as can be handled efficiently by computer. The Coulomb radius is calculated from the formula (BW52, p. 205)

$$R^{-1}_{\text{coulomb}} = \frac{5}{6N}\int_0^\infty \{\;[\sum_{i=o}^{k} c_i\; e^{-\lambda_i a}\;]^2\; F(a)da \qquad (16)$$

and the mass root-mean-square radius (L68) from

$$R^2_{r.m.s.} = \frac{1}{3N} \int_0^\infty a^3 \left[\sum_{i=0}^{k} c_i \, d^{-\lambda_i a} \right]^2 F(a)da \qquad (17)$$

APPENDIX C

TRACELESS SYMMETRIC TENSORS

When we decompose the three-body triton wave function into components with explicit two-body LSJ dependence, we make use of the fact that the linearly independent components of a traceless symmetric tensor of rank L form a basis for an irreducible representation of dimension 2L+1. For convenience, we enumerate some of our definitions, notations, and identities below. The number of subscripts is the rank of the tensor. We assume the Einstein summation convention.

$$T_i(a) = a_i$$

$$T_{ij}(a,b) = \frac{1}{2}\{a_i b_j + a_j b_i - \frac{2}{3}\delta_{ij}\ (\vec{a}\cdot\vec{b})\}$$

$$\begin{aligned} T_{ijk}(a,b,c) = \frac{1}{3}\{&T_{ij}(a,b)c_k + T_{jk}(a,b)c_i + T_{ki}(a,b)c_j \\ &- \frac{2}{5}[\delta_{ij}\ T_{ks}(a,b)c_s + \delta_{jk}\ T_{is}(a,b)c_s \\ &+ \delta_{ki}\ T_{js}(a,b)c_s\ ]\} \end{aligned}$$

$$\begin{aligned} T_{ijk\ell}(a,b,c,d) = \frac{1}{4}\{&T_{ijk}(a,b,c)d_\ell + T_{ijk\ell}(a,b,c)d_i \\ &+ T_{k\ell i}(a,b,c)d_j + T_{\ell ij}(a,b,c)d_k \\ &- \frac{2}{7}[\delta_{ij}\ T_{k\ell s}(a,b,c)d_s + \delta_{jk}\ T_{\ell is}(a,b,c)d_s \end{aligned}$$

$$+ \delta_{\ell i} T_{jks}(a,b,c)d_s + \delta_{ik} T_{j\ell s}(a,b,c)d_s$$

$$+ \delta_{j\ell} T_{iks}(a,b,c)d_s + \delta_{k\ell} T_{ijs}(a,b,c)d_s]\}$$

The trend is evident from the above expressions; higher rank tensors can be written down and checked to see whether they are symmetric and traceless.

Tensors derived from vectors, one of which is a cross product, can be written as

$$T_{ij}(a,\ a \times b) = \frac{1}{2}\{T_{ik}(a,a)\varepsilon_{jk\ell}b_\ell + T_{jk}(a,a)\varepsilon_{ik\ell}b_\ell\}$$

$$T_{ijk}(a,a,\ a \times b) = \frac{1}{3}\{T_{ij\ell}(a,a,a)\varepsilon_{k\ell m}\ b_m$$

$$+ T_{jk\ell}(a,a,a)\varepsilon_{i\ell m}b_m$$

$$+ T_{ki\ell}(a,a,a)\varepsilon_{j\ell m}b_m$$

$$T_{ijk\ell}(a,a,a,\ a \times b) = \frac{1}{4}\{T_{ijkm}(a,a,a,a)\varepsilon_{\ell mn}b_n$$

$$+ T_{jk\ell m}(a,a,a,a)\varepsilon_{imn}b_n$$

$$+ T_{i\ell km}(a,a,a,a)\varepsilon_{jmn}b_n$$

$$+ T_{\ell ijm}(a,a,a,a)\varepsilon_{kmn}b_n$$

where $\varepsilon_{\ell mn}$ is the permutation symbol (S60, chapter VI). Denoting the rank of the tensor by a bracketed superscript and the contraction of all subscripts by a dot, we write the following useful identities.

$$T^{(1)}(a)\cdot T^{(1)}(b) = (\vec{a}\cdot\vec{b})$$

$$T^{(2)}(a)\cdot T^{(2)}(b) = (\vec{a}\cdot\vec{b})^2 - \frac{1}{3}a^2b^2$$

$$T^{(3)}(a)\cdot T^{(3)}(b) = (\vec{a}\cdot\vec{b})^3 - \frac{3}{5}a^2b^2(\vec{a}\cdot\vec{b})$$

$$T^{(4)}(a)\cdot T^{(4)}(b) = (\vec{a}\cdot\vec{b})^4 - \frac{6}{7}a^2b^2(\vec{a}\cdot\vec{b})^2 + \frac{3}{35}a^4b^4$$

$$T^{(5)}(a)\cdot T^{(5)}(b) = (\vec{a}\cdot\vec{b})^5 - \frac{10}{9}a^2b^2(\vec{a}\cdot\vec{b})^3 + \frac{5}{21}a^4b^4(\vec{a}\cdot\vec{b})$$

$$T^{(6)}(a)\cdot T^{(6)}(b) = (\vec{a}\cdot\vec{b})^6 - \frac{15}{11}a^2b^2(\vec{a}\cdot\vec{b})^4$$

$$+ \frac{5}{11}a^4b^4(\vec{a}\cdot\vec{b})^2 - \frac{5}{231}a^6b^6$$

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