

REACTION MATRICES FOR FINITE NUCLEI

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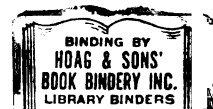
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ABSTRACT

REACTION MATRICES FOR FINITE NUCLEI

by David V. Grillot

A method for calculating the reaction matrix elements of a closed-shell nucleus is discussed. An improved treatment of the Pauli operator is proposed, and accurate solutions of the Bethe-Goldstone are obtained for the coupled and uncoupled integro-differential equations. The solutions are used to obtain the first order binding energy of ^{16}O using the Hamada-Johnston and Brueckner-Gammel-Thaler potentials. The results indicate that the Hamada-Johnston potential gives too little binding and possible ways of improving the binding energy calculations are discussed. The reaction matrix is examined as a function of the single particle energies. It was found that the $^3\text{S}_1$ states are very sensitive to the choice of single particle energies; whereas, the $^1\text{S}_0$ states are relatively insensitive to this choice. Calculated singularities of the reaction matrix are also reported for both the $^1\text{S}_0$ and $^3\text{S}_1$ states.

REACTION MATRICES FOR FINITE NUCLEI

by

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CHAPTER I

INTRODUCTION

The initial attempts to classify and explain nuclear structure relied upon certain models, viz., the shell-model and the collective model. These models and generalizations of these models had some moderate successes; however, there were also some notable failures.

The initial attempts to overcome the shortcomings of these models and to develop a unified nuclear perturbation theory were made by Brueckner,¹ Bethe, and Goldstone,² One of the major difficulties in the development of the nuclear perturbation theory was the strong nature of the nucleon-nucleon potential, v , which when used in the conventional perturbation theory gives rise to divergent matrix elements. The many body perturbation theory shows that the infinite matrix elements, $\langle \phi | v | \phi \rangle$, should be replaced by the finite matrix elements, $\langle \phi | \tau | \phi \rangle$, where t is a two body operator defined by

$$t_{12} = v_{12} - v_{12} \frac{Q}{E} t_{12}, \quad (1)$$

¹K. A. Brueckner and J. L. Gammel, Phys. Rev. 109 (1958) 1023, this work lists all earlier references.

²H. A. Bethe and J. Goldstone, Proc. Roy. Soc. (London), 238A (1957) 551.

and

$$\tau_{12} \phi = \sqrt{12} \psi \quad (2)$$

In these expressions Q is the Pauli projection operator which prevents two interacting nucleons from scattering into states occupied by other spectator nucleons. The energy denominator, e , is the difference between the energies of the pair of nucleons in their excited intermediate states and their initial states. Considerable confusion exists in the literature about the precise nature of the energy denominator. The current belief is that this energy denominator should be comprised of Hartree-Fock (HF) single particle energies.³

The first attempts to solve equations (1) and (2) were carried out for nuclear matter, i. e., an artificial nucleus of infinite extent in which the Coulomb effects are neglected. One of the major simplifications for nuclear matter is that the intermediate state wave functions are plane waves. This is possible due to the translational invariance of nuclear matter. Another simplification for nuclear matter is that the intermediate state energies are the energies of free particles. Even with these simplifications, the calculations of the binding energy

³ M. K. Pal and A. P. Stamp, Phys. Rev. 158 (1967) 924.

of nuclear matter have oscillated throughout the past ten years and are still in a state of flux.

Despite the uncertainties of the nuclear matter results, one of the more instructive conclusions to be shown is that the many body theory reduces in a certain approximation to the earlier shell model. This was shown to be the case by Gomes, Walecka, and Weisskopf.⁴ Their calculation using the t-matrix formalism of references 1, 2 showed in a convincing manner that, (a) the many body effects fundamentally alter the correlated motion of a pair of nucleons such that the perturbed wave function heals to the unperturbed wave function and (b) the hard core potential could be treated in a consistent non-divergent manner. The first conclusion is a result fundamental to both nuclear matter and finite nuclei, and the "healing" of the correlated wave function to the unperturbed wave function can be used either as a calculational tool or can be viewed as a qualitative test for proposed two nucleon wave functions.

The transition from early nuclear matter calculations using the t-matrix formalism to the present day calculations for finite

⁴L. C. Gomes, J. D. Walecka, and V. F. Weisskopf, Ann. Phys. 3(1958) 241.

nuclei has proceeded quite slowly. The slowness of this transition is due basically to the fact that the simplifying assumptions of intermediate state energies and wave functions cannot be carried over readily to finite nuclei. In fact at the present time there is no firm basis for choosing the intermediate state energies and it will be shown in Chapter III that the t-matrix elements are dependent on the energy denominator. Moreover, in finite nuclei the Pauli operator is difficult to handle because the bookkeeping devices, viz, Racah coefficients and Moshinsky brackets⁵ are cumbersome to treat.

As has been stressed by several authors^{3, 6} the rigorously correct calculational procedure is a doubly self-consistent computation. That is, using equation (1), a set of t-matrices are computed with some realistic nucleon-nucleon potential. Using these initial t-matrices, a self-consistent HF calculation is performed. The HF calculation generates a set of single particle energies and wave functions. These single particle energies and wave functions are then used to recalculate a new set of t-matrices. The double iterative

⁵T. A. Brody and M. Moshinsky, Tables of Transformation Brackets (Monografias del Institute de Fisica, Mexico, 1960).

⁶K. Kumar, Perturbation Theory and the Nuclear Many Body Problem (North Holland Publishing Co., Amsterdam, 1962).

procedure is then repeated until a self-consistent set of single particle energies and wave functions is obtained. Even using high speed computers the problem of achieving double self-consistency is only now becoming feasible.

In order to avoid the above-mentioned complexities several simplifying assumptions are usually introduced ^{7, 8, 9}, which will be maintained in the present paper. The first assumption is that the intermediate HF wave functions are replaced by harmonic oscillator wave functions. This approximation has been discussed by Kuo and Brown ⁷ who argue that the results of HF calculations ¹⁰ give wave functions which are similar to harmonic oscillator wave functions. The next major assumption is that the Bethe-Goldstone (BG) wave function, ψ , can be separated into an unperturbed center-of-mass wave function and a perturbed relative wave function. There is no justification for this assumption due to the nonlocality of the Pauli operator, but unless this assumption is made the BG equation

⁷ T. T. S. Kuo, and G. E. Brown, Nucl. phys., 85 (1966) 40.

⁸ C. W. Wong, Nucl. Phys. A91 (1967) 399.

⁹ A. D. Mackellar PhD Thesis, Texas A and M University, January 1966 (Unpublished).

¹⁰ L. Kelson and C. A. Levinson, Phys. Rev. 134 (1964) B269.

is insoluble. The retention of this approximation will be necessary until a suitable method of solving directly the two-body BG equation is devised. The final assumption concerns the nature of the intermediate state energies. As mentioned earlier there is no clear basis for choosing these energies; however, two choices are now popular. The first choice is based on nuclear matter results and uses plane waves; the second choice is to use harmonic oscillator energies. Both of these choices are questionable, and in this paper the harmonic oscillator is chosen.

Before the complete self-consistent problem is attempted it is necessary that accurate solutions of equation (1) be obtained. Unless one has confidence in these fundamental solutions it seems unwarranted to proceed with the larger calculation.

Recently there have been several convincing solutions to equation (1). The more notable of these have used the reference spectrum method,¹¹ the separation method,¹² and the Eden-Emery method.¹³ Kuo and Brown⁷ have applied the first two methods to

¹¹H. A. Bethe, B. H. Brandow and A. G. Petshek, Phys. Rev. 129 (1963) 225.

¹²S. A. Moszkowski and B. L. Scott, Ann. Phys. 11 (1960) 65.

¹³R. J. Eden, V. J. Emery and S. Sampanthar, Proc. Roy. Soc. (London) A253 (1959) 186.

the excited state spectrum of ^{18}F and ^{18}O and the binding energy of ^{16}O . Mackellar⁹ has used the latter method to obtain the binding energy of ^{16}O .

Both the separation method and the reference spectrum method use a perturbation expansion of the t-matrix which in the first approximation neglects the Pauli operator. The Pauli operator occurs in the perturbation expansion and is ultimately calculated by using the angle average Pauli operator which was originally used for nuclear matter. Recently Wong⁸ has improved the Kuo-Brown treatment of the Pauli operator.

The separation method and the reference spectrum method differ basically in the choice of the first order t-matrix. In the separation method, which was initially used by Moszkowski and Scott¹² for nuclear matter, one assumes that the potential can be separated into a short range and a long range part. The separation distance is chosen such that the short range attraction in some sense cancels the repulsive hard core part of the potential. Then one is left with the problem of evaluating the long range part of the potential via the perturbation expansion for the reaction matrix. There are several minor assumptions such as averages of state

dependent separation distances, but it is believed that these corrections are small.¹⁴

The reference spectrum method was originally suggested by Bethe, Brandow, and Petchek¹¹ for nuclear matter. This method has particular utility for the odd state repulsive potentials because the concept of a separation distance is meaningless for these states. In this method the first order t-matrix neglects the Pauli operator and approximates the intermediate state energies with the free particle energies. With these approximations one gets an inhomogeneous differential equation for the first order t-matrix. The higher order corrections to the reaction matrix are then calculated in a manner analogous to the separation method.

In both methods the question of convergence of the perturbation expansion is made plausible by explicitly showing that higher order terms are small.

The third method was originally suggested by Eden and Emery in a series of papers,¹³ and some calculations were performed using questionable numerical approximations. Mackellar⁹ has recently redone the calculations in a precise manner for ^{16}O using several different nucleon-nucleon

¹⁴T. T. S. Kuo, to be published.

potentials. There are two basic approximations in this approach to the problem which make the calculations possible. The first is to observe that a tenable approximation exists for the Pauli operator based on the unique characteristics of the harmonic oscillator wave functions. The final effect of this approximation in ^{16}O is to forbid scattering into one allowed state and permit scattering into a set of forbidden states. Despite these restrictions the method does include the essential features of the Pauli operator.

The second approximation is the treatment of the HF self-consistency condition. By introducing a state dependent potential for the initial state energies, it is possible to obtain approximate self-consistency for the BG wave function.

The overall method deviates considerably from the framework of the nuclear many body theory, and despite its ability to predict nuclear binding energies it is an artificial approach to the problem.

In the present paper some of the above-mentioned approximations are avoided. In particular it is shown that it is unnecessary to construct a perturbation expansion for the t-matrix since equation (1) can be solved exactly. At first glance this appears to be an involved calculation, but in actuality the calculation is simpler and avoids any question of convergence of the perturbation

series. Moreover, there is no necessity of calculating state dependent separation distances.

In addition to this exact solution, it will be shown in Chapter II that it is possible to incorporate an improved treatment of the Pauli operator. This improved treatment of the Pauli operator and the exact solution of equation (1) should increase the reliability of the t-matrix elements for finite nuclei, and it is anticipated that one could now proceed with the full self-consistent problem.

CHAPTER II

FORMULATION OF THE PROBLEM

1. General Development

Rather than solving equation (1) of Chapter I, the standard procedure is to calculate the two body correlated wave function, ψ . By combining equations (1) and (2) of Chapter I, the following is obtained for the BG wave function:

$$\psi = \phi + \frac{Q}{E} \mathcal{N} \psi \quad (1)$$

Or in terms of the wave operator

$$\mathcal{N} = 1 + \frac{Q}{E} \mathcal{N}$$

Once equation (1) is solved, the diagonal and off-diagonal reaction matrix elements are determined from

$$\langle \phi | t | \phi \rangle = \langle \phi | \mathcal{N} | \psi \rangle \quad (2)$$

which is a finite quantity since ψ vanishes in that region where the potential, v , has an infinite hard core.

In Appendix A a detailed analysis of the hard core shows that the hard core contribution to the t-matrix is given approximately by $\phi \frac{d\psi}{dr} \big|_{r=r_c}$. This contribution has been added to all matrix elements in equation (2).

The task is to solve equation (1) which is the Bethe-Goldstone (BG) equation in as exact manner as possible. For complete generality the BG equation is written in the j-j representation even though this generality is not needed for closed-shell nuclei. In this representation the BG equation is

$$\begin{aligned} \Omega |(l_1 a_1) j_1 (l_2 a_2) j_2 J M_T M_T m_1 m_2\rangle &= |(l_1 a_1) j_1 (l_2 a_2) j_2 J M_T M_T m_1 m_2\rangle \\ &+ \frac{1}{2} \sum_{\substack{\text{UNOCCUPIED} \\ n'_1 l'_1 j'_1 J'_1 M'_1 T'_1 \\ n'_2 l'_2 j'_2 J'_2 M'_2 T'_2}} (1 + \delta_{n'_1 l'_1 j'_1, n'_2 l'_2 j'_2}) |(l'_1 a'_1) j'_1 (l'_2 a'_2) j'_2 J'_1 M'_1 T'_1 m'_1 m'_2\rangle \\ &\times \frac{\langle (l'_1 a'_1) j'_1 (l'_2 a'_2) j'_2 J'_1 M'_1 T'_1 m'_1 m'_2 | V \Omega |(l_1 a_1) j_1 (l_2 a_2) j_2 J M_T M_T m_1 m_2\rangle}{\epsilon_{n_1 l_1 j_1} + \epsilon_{n_2 l_2 j_2} - \epsilon_{n'_1 l'_1 j'_1} - \epsilon_{n'_2 l'_2 j'_2}} \end{aligned} \quad (3)$$

where $n l j$ designate the single particle quantum numbers, $\epsilon_{n l j}$ are the initial state self-consistent energies, and $\epsilon_{n' l' j'}$ are the energies of the intermediate states. The summation in equation (3) is carried out over all initially unoccupied states and in principle these states should be the self-consistent HF single particle states. ⁶

Since the complete self-consistent problem, i. e., the problem of doing a self-consistent HF calculation in conjunction with a self-consistent treatment of the BG equation, is an extremely involved computational exercise, the approximation of replacing the intermediate state single particle wave functions by harmonic oscillator wave functions is made. The initial state energies, which should also be determined in a self-consistent manner, are varied over a wide range of physically interesting values. For the final calculation of the t-matrix elements, the initial single particle energies are obtained from Hartree-Fock calculations.³ The intermediate state energies $\epsilon_{n_1 l_1 j_1} + \epsilon_{n_2 l_2 j_2}$, are chosen to be harmonic oscillator energies. Based on these considerations the problem of double self-consistency as discussed by Pal and Stamp³ is circumvented.

Due to the nonlocality of the Pauli operator the BG equation is not separable into relative and center-of-mass coordinates. Therefore, the major approximation of this paper will be to assume that the BG wave function, ψ , can be separated into a perturbed relative wave function and an unperturbed center-of-mass wave function.

Similar assumptions are made for the initial state energies

$$\epsilon_1 + \epsilon_2. \text{ That is } \epsilon_{n_1 l_1 j_1} + \epsilon_{n_2 l_2 j_2} = E_{nljS}^{\text{rel.}} + E_{NL}^{\text{C.M.}}$$

where $nljS$ are quantum numbers of the relative state and NL are center-of-mass quantum numbers.

Using these assumptions the BG equation can be reduced to an integro-differential equation by performing the following algebraic manipulations:

(1) Operate with

$$\epsilon_{m_1 l_1 j_1} + \epsilon_{m_2 l_2 j_2} - H_0 = E_{nlj}^{rel.} + E_{NL}^{c.M.} - H_0^{rel.} - H_0^{c.M.} \quad (4)$$

where H_0 is the harmonic oscillator Hamiltonian. (2) Change the sum over the unoccupied states to one minus the sum over occupied states. (3) Use the standard transformation for the perturbed and unperturbed states, viz.,

$$\begin{aligned} |(l_1, a_1) j_1, (l_2, a_2) j_2, JM_T, TM_T, m_1, m_2\rangle &= [2(1 + \delta_{m_1 l_1 j_1, m_2 l_2 j_2})]^{-1} \\ &\times \sum_{s \wedge m \wedge NL} T_{s \wedge J}^{l_1 l_2 j_1 j_2} \langle m l NL, 1 | m_1 l_1 m_2 l_2 \rangle [1 - (-1)^{l+s+\pi}] \\ &\times \sum_j \Lambda_{JLA}^{psj} \sum_{m_j m_L} C(j L m_j m_L | JM_T) |L M_L N\rangle | (ps) j m_j n \rangle | TM_T \rangle \quad (5) \end{aligned}$$

where

$$T_{SAJ}^{l_1 j_1 l_2 j_2} = \sqrt{(2S+1)(2\Lambda+1)(2j_1+1)(2j_2+1)} \begin{Bmatrix} l_1 & l_2 & j_1 \\ l_2 & l_1 & j_2 \\ \Lambda & S & J \end{Bmatrix} \quad (6)$$

and

$$\Lambda_{JLA}^{lSj} = (-1)^{S+L+j+\Lambda} \begin{Bmatrix} l & S & j \\ J & L & \Lambda \end{Bmatrix} \quad (7)$$

In these expressions the angular momentum j_1 and j_2 couple to a total angular momentum, J . The spin of the two nucleons is S , and l , L , and Λ are the relative, center-of-mass, and total orbital angular momentum respectively. The T -coefficients are the transformation coefficients from j - j to L - S coupling. Λ_{JLA}^{lSj} is the recoupling coefficient of l and S to a total relative angular momentum, j . And the bracket $\langle n_1 n_2 L, \Lambda | n_1 l_1 n_2 l_2 \rangle$ is the Brody-Moshinsky transformation bracket.⁵ (4) Eliminate the center-of-mass energy by using $(E_{NL}^{C.M.} - H_0^{C.M.}) | LM_L N \rangle = 0$. (5) Take the scalar product of the transformed equation with $\langle LM_L N |$ and $\langle TM_T |$. (6) Assume that the interaction is diagonal in S , T , M_T , j and m_j .

(7) Finally for closed-shell nuclei use the orthogonality properties of the T-coefficients,¹⁵ viz., $\sum_{j_1 j_2} T_{S \Lambda J}^{1 1 2 j_1 j_2} T_{S' \Lambda' J}^{1 1 2 j_1 j_2} = \delta_{SS'} \delta_{\Lambda \Lambda'}$
 After performing these operations and using the properties of the Clebsch-Gordan coefficients, the following equation is obtained:

$$\begin{aligned}
 (E_{nljs} - H_0^{rel})(\Omega - 1) |(ls)j m_j m\rangle &= \nu \Omega |(ls)j m_j m\rangle \\
 &- \sum_{\substack{\text{OCCUPIED} \\ n'l'm_l'j'm_j'}} \frac{1}{4} \sum_{n'l'm_l'j'm_j'} \langle n'l'NL, \Lambda_0 | n'l'm_l'j'm_j' \rangle \langle n'l'm_l'j'm_j' | n'l'NL, \Lambda_0 \rangle \\
 &\times [1 - (-1)^{l'+s+\pi}] [1 - (-1)^{l'+s+\pi}] \Lambda_{jL\Lambda_0}^{l'sj} C(jL m_j m_l | J_0 M_0) \\
 &\times \sum_j \Lambda_{jL\Lambda_0}^{l'sj} C(jL m_j m_l | J_0 M_0) |(l's)j m_j m\rangle \langle (l's)j m_j m | \nu \Omega |(ls)j m_j m\rangle
 \end{aligned} \quad (8)$$

This equation is valid for either $l=j$ or $l=j-1$.

2. Singlet and Triplet $l=j$ states.

In this section only the case where $l=j$ will be considered.

Define

$$\langle \bar{\alpha} | (ls)j m_j m \rangle = \frac{R_{nl}(\alpha)}{\alpha} \chi_{jls}^{m_j} \quad (9)$$

¹⁵A. DeShalit and I. Talmi, Nuclear Structure Theory (Academic Press Inc., New York, 1963).

and

$$\langle \tilde{r} | \Omega | (ls) j m_j n \rangle = \frac{u_{mljs}(\tilde{r})}{\tilde{r}} y_{jls}^{m_j} \quad (10)$$

where $y_{jls}^{m_j}$ is the standard angular momentum function which has been defined elsewhere.¹⁶ Also introduce a dimensionless variable

$$\rho = r/b, \quad (b = \sqrt{\hbar / m\omega}) .$$

Then after taking the scalar product $y_{jls}^{m_j}$ with equation (8), summing both sides over m_j and m_L , performing the sum over M_{J_0} and J_0 , and using the implicit energy relations of the Brody-Moshinsky bracket,⁵ the following expression is obtained:

$$\begin{aligned} & \left[\lambda_{mljs} + \frac{d^2}{ds^2} - \frac{l(l+1)}{s^2} - s^2 - \frac{2}{\hbar\omega} \langle y_{jls} | N | y_{jls} \rangle \right] u_{mljs}(s) \\ &= \left[\lambda_{mljs} - \lambda_{ml}^0 \right] R_{ml}^{(s)} \langle R_{ml} | u_{mljs} \rangle \\ & - \sum_{\substack{\text{OCCUPIED} \\ m_1^0, l_1^0, m_2^0, l_2^0}} R_{m_1 l_1}^{(s)} \frac{2}{\hbar\omega} \int_0^\infty R_{m_2 l_2}^{(s')} \langle y_{jls} | N | y_{jls} \rangle u_{mljs}(s') ds' \\ & \times \left\{ [(2L+1)(2l+1)]^{-1} \sum_{\lambda_0} (2\lambda_0+1) \left| \langle m_0, \lambda_0, \lambda_0 | m_1^0, l_1^0, m_2^0, l_2^0 \rangle \right|^2 \right\} \end{aligned} \quad (12)$$

¹⁶M. A. Preston, Physics of the Nucleus (Addison-Wesley Publishing Co., Reading, Massachusetts, 1962).

where $n_o = (2n_1^o + 1_1^o + 2n_2^o + 1_2^o - 2N-L-1)/2$, $\lambda_{nljS} = \frac{2}{\hbar\omega} E_{nljS}^{\text{rel.}}$, and $\lambda_{nl}^o = 2(2n+1) + 3$.

Equation (12) is the final reduced form of the BG equation which has to be solved. It should be emphasized that the only major approximation which has been made in deriving equation (12) is the separability of the BG wave function.

By explicitly writing out equation (12) it becomes obvious that the form of this equation is identical to the equation derived by Eden and Emery.¹³ However, there are several major differences. As is well-known⁹ the Eden-Emery approximation incorrectly includes and excludes scattering into certain intermediate states. This approximation manifests itself in the number of terms in the sum in the reduced equation. Also, equal weights are assigned to all intermediate occupied states. In the present treatment of the BG equation both of these difficulties are corrected. That is, each intermediate state is multiplied by the appropriate weighting coefficient and the summation is over the proper number of terms. In the Eden-Emery method there is no clear prescription for extending the method to nuclei other than ¹⁶O. It is now apparent how equation (12) can be extended to any closed-shell nucleus. In addition the Eden-Emery energy denominator differs from the present formulation.

3. Triplet $l=j-1$ states.

In this section only the case where $l=j-1$ is the dominant solution will be considered.

Define

$$\langle \pi | (lS) j m_j n \rangle = \frac{R_{nl}(\pi)}{\pi} y_{jls}^{m_j}(\theta, \phi) \quad (13)$$

and

$$\langle \pi | \Omega | (lS) j m_j n \rangle = \frac{u_{nljS}(\pi)}{\pi} y_{jls}^{m_j}(\theta, \phi) + \frac{w_{n'l'jS}}{\pi} y_{j'l'S}^{m_j}(\theta, \phi) \quad (14)$$

where u_{nljS} is the $l=j-1$ component of the solution and $w_{n'l'jS}$ is the $l'=j+1$ component of the solution. When u_{nljS} is the dominant solution, this implies that the unperturbed state is an $l=j-1$ state.

The procedure used in deriving the relevant reduced coupled equations is, in principle, the same as that used for the uncoupled equations. Starting with equation (8), the scalar product with first y_{jls} and then $y_{j'l'S}$ is taken. This leads to two equations which are summed over m_j and m_L . The summation over M_{J_0} and J_0 can then be performed and if the implicit energy relations of the Brody-Moshinsky brackets are used, the following expressions are obtained:

$$\begin{aligned}
& \left[\lambda_{mljs} + \frac{J^2}{4f^2} - \frac{l(l+1)}{f^2} - f^2 - \frac{2}{\hbar\omega} \langle y_{jls} | v | y_{jls} \rangle \right] u_{mljs}^{(f)} \\
& - \frac{2}{\hbar\omega} \langle y_{jls} | v | y_{jls} \rangle \omega_{ml'js}^{(f)} = [\lambda_{mljs} - \lambda_{ml}^0] R_{ml}^{(f)} \langle R_{ml} | u_{mljs} \rangle \\
\end{aligned} \tag{15a}$$

$$\begin{aligned}
& - \sum_{\substack{\text{OCCUPIED} \\ m_0' l_0' m_2' l_2'}} R_{m_0' l_0'}^{(f')} \frac{2}{\hbar\omega} \int_0^\infty R_{m_0 l}^{(f')} \left[\langle y_{jls} | v | y_{jls} \rangle u_{mljs}^{(f)} + \langle y_{jls} | v | y_{jls} \rangle \omega_{ml'js}^{(f)} \right] ds' \\
& \times \left\{ [(2L+1)(2l+1)]^{-1} \sum_{\Lambda_0} (2\Lambda_0+1) |\langle m_0 l N L, \Lambda_0 | m_0' l_0' m_2' l_2' \rangle|^2 \right\}
\end{aligned}$$

and

$$\begin{aligned}
& \left[\lambda_{mljs} + \frac{J^2}{4f^2} - \frac{l'(l'+1)}{f^2} - f^2 - \frac{2}{\hbar\omega} \langle y_{jls} | v | y_{jls} \rangle \right] \omega_{ml'js}^{(f)} \\
& - \frac{2}{\hbar\omega} \langle y_{jls} | v | y_{jls} \rangle u_{mljs}^{(f)} = \\
& - \sum_{\substack{\text{OCCUPIED} \\ m_0' l_0' m_2' l_2'}} R_{m_0' l_0'}^{(f')} \frac{2}{\hbar\omega} \int_0^\infty R_{m_0 l}^{(f')} \left[\langle y_{jls} | v | y_{jls} \rangle \omega_{ml'js}^{(f)} + \langle y_{jls} | v | y_{jls} \rangle u_{mljs}^{(f)} \right] ds' \\
& \times \left\{ [(2L+1)(2l'+1)]^{-1} \sum_{\Lambda_0} (2\Lambda_0+1) |\langle m_0' l_0' N L, \Lambda_0 | m_0 l m_2 l_2 \rangle|^2 \right\}
\end{aligned} \tag{15b}$$

where

$$n_o = (2n_1^o + l_1^o + 2n_2^o + l_2^o - 2N - L - 1)/2 \quad (16)$$

$$n_o' = (2n_1^o + l_2^o + 2n_2^o + l_2^o - 2N - L - 1')/2 \quad (17)$$

Comments identical to those following equation (12) about the comparison of these equations with those of Eden and Emery can also be made.

4. Approximate Solution of BG Equation

Although the approach discussed in this section has been superseded by the formulations of the previous sections, it is instructive to analyze the BG equation when the Pauli operator is completely ignored. For this situation a model is assumed in which two nucleons interact through the nucleon-nucleon potential while the spectator nucleons affect the interacting particles only through a spherically symmetric potential which is chosen to be a harmonic oscillator potential. The two particle Hamiltonian is then $H=H_o+v$, and the wave function satisfies the eigenvalue equation

$$(E - H_o - v) \psi^o = 0 \quad (18)$$

Because of the properties of the harmonic oscillator, the total Hamiltonian separates readily into the sum of center-of-mass and relative coordinates. The equation for the center-of-mass is

$$(E^{c.m.} - H_0^{c.m.}) \psi_{c.m.} = 0 \quad (19)$$

and is readily solved analytically. The relative equation in terms of the dimensionless variable ρ is

$$\left[\lambda_{nljs} + \frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} - \rho^2 - \frac{2}{\hbar\omega} \langle y_{jls} | r | y_{jls} \rangle \right] u_{nljs}^0(\rho) = 0 \quad (20)$$

for the uncoupled $l=j$ states, and for the coupled $l=j-1$ states,

$$\left[\lambda_{nljs} + \frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} - \rho^2 - \frac{2}{\hbar\omega} \langle y_{jls} | r | y_{jls} \rangle \right] u_{nljs}^0(\rho) - \frac{2}{\hbar\omega} \langle y_{jls} | r | y_{j's} \rangle \omega_{n'l'j's}^0 = 0 \quad (21a)$$

and

$$\left[\lambda_{nljs} + \frac{j^2}{4s^2} - \frac{l'(l'+1)}{s^2} - j^2 - \frac{2}{\hbar\omega} \langle \chi_{j,l's} | \nu | \chi_{j,l's} \rangle \omega_{nlj's}^{(p)} \right. \\ \left. - \frac{2}{\hbar\omega} \langle \chi_{j,l's} | \nu | \chi_{j,l's} \rangle \omega_{nlj's}^{(p)} = 0 \right] \quad (21b)$$

these equations which ignore the Pauli operator should be compared with equations 12, 15a and 15b which include the Pauli operator.

Although the form of the eigenvalue equation is considerably different from the correct form of the BG equation, it was originally thought that the eigenfunctions would be reasonably good approximations to the BG wave functions particularly for the higher angular momentum states. A priori it is difficult to assess the severity of neglecting the Pauli operator. Dawson, Talmi and Walecka,¹⁷ based on some crude estimates of the effect of the Pauli operator in ¹⁸O, showed that the effect of neglecting the Pauli operator in the ¹S₀ states would result in about 10% error. It was hoped that the same would be true for the troublesome ³S₁ states. The present paper will show in the next chapter that for the ¹S₀ states their estimate

¹⁷J. F. Dawson, I. Talmi, and J. D. Walecka, Ann. Phys. 18 (1962), 339.

of the error is reasonable. However, for the 3S_1 states one is not quite so fortunate, and it is imperative that the Pauli operator be taken into account. Moreover, in order to obtain decent values for the binding energy of ^{16}O it is necessary to include the Pauli operator.

In addition to the above quantitative considerations the qualitative comparisons of the solutions with and without the Pauli operator demonstrates in a dramatic fashion the effect of the Pauli operator on the nuclear wave function.

CHAPTER III

NUMERICAL RESULTS

A computer program has been written to solve the coupled and uncoupled integro-differential equations exactly, i. e., equations 12 and 15 of Chapter II. The numerical technique used to solve these equations is discussed in detail in Appendix B. The numerical accuracy required for the wave function, u , is $\delta u/u < .005$ where

δu is the computed change in the wave function at the end of each iteration. Usually three iterations were sufficient for convergence. The method of solution was quite efficient, and ultimately it was faster to solve the full BG equation than the related eigenvalue problem. Disregarding compilation time, the computer time required to calculate one state and its off-diagonal matrix elements was 30 seconds and 60 seconds for the uncoupled and coupled states respectively using an IBM - 360 Model 50 computer.

The nucleus of interest in this calculation was ^{16}O , but the method developed has equal applicability to other closed-shell nuclei. For ^{16}O the summation in equations (12) and (15) is carried out over the $0s$ and $0p$ shell. For other closed-shell nuclei it is necessary to alter the range of this summation accordingly.

In solving equations (12) and (15), three pieces of information are needed: a phenomenological nucleon-nucleon potential, a set of HF single particle energies, and an oscillator parameter, $\hbar\omega$.

The equations were solved using both the Hamada-Johnston¹⁸ (HJ) and the Brueckner-Gammel-Thaler¹⁹ (BGT) potentials. Both of these potentials contain a hard-core, tensor force and spin-orbit force. In addition the HJ potential contains a quadratic spin-orbit force. The properties and parameters of these potentials are given in Appendix C.

The values of the HF single particle energies were -40 and -18 MeV for the os and op states respectively. These were the values calculated by Pal and Stamp³ and should be correct to within 5MeV. It should be realized that these values will be altered somewhat when the doubly self-consistent calculation is performed. Since there is doubt concerning the specific dependence of the t-matrix on the initial state single particle energies a detailed examination of this dependence has been performed for the 1S_0 and 3S_1 states.

¹⁸T. Hamada and I. D. Johnston, Nucl. Phys. 34 (1962) 382.

¹⁹K. A. Brueckner, J. L. Gammel and R. M. Thaler, Phys. Rev. 109 (1958) 1023.

The oscillator parameter used was based on electron scattering data²⁰ which indicates that the value of $\hbar\omega$ for ^{16}O should be between 13 and 15 MeV. The t-matrix elements were calculated using three values of $\hbar\omega$, viz., 13.35, 14.5, and 15.5 MeV. Ultimately more values of $\hbar\omega$ were needed to clearly define a minimum in the B.E. /A versus $\hbar\omega$ curve.

With these pieces of information the first equation solved was equation (20), i. e., the eigenvalue equation which neglects the Pauli operator. This equation was solved for all angular momentum states less than 3 and for both the singlet and triplet states. The resulting $^1\text{S}_0$ relative wave function, u_{00}^0 , is plotted in Figure 1 and is compared to the unperturbed harmonic oscillator, R_{00} . The important qualitative feature to be noted is that there is no healing of the wave function u_{00}^0 onto the unperturbed solution. In this situation, the scattering of the two nucleons inside the harmonic oscillator potential can be viewed as a real scattering process in which the final wave function has undergone a phase shift.

Figure 1 should be compared directly with Figure 2 in which the perturbed wave function, u_{00} , is plotted. Here u_{00} is the $^1\text{S}_0$ solution of equation (12) which includes the Pauli projection operator.

²⁰L. R. B. Elton, Nuclear Sizes (Oxford University Press, 1961).

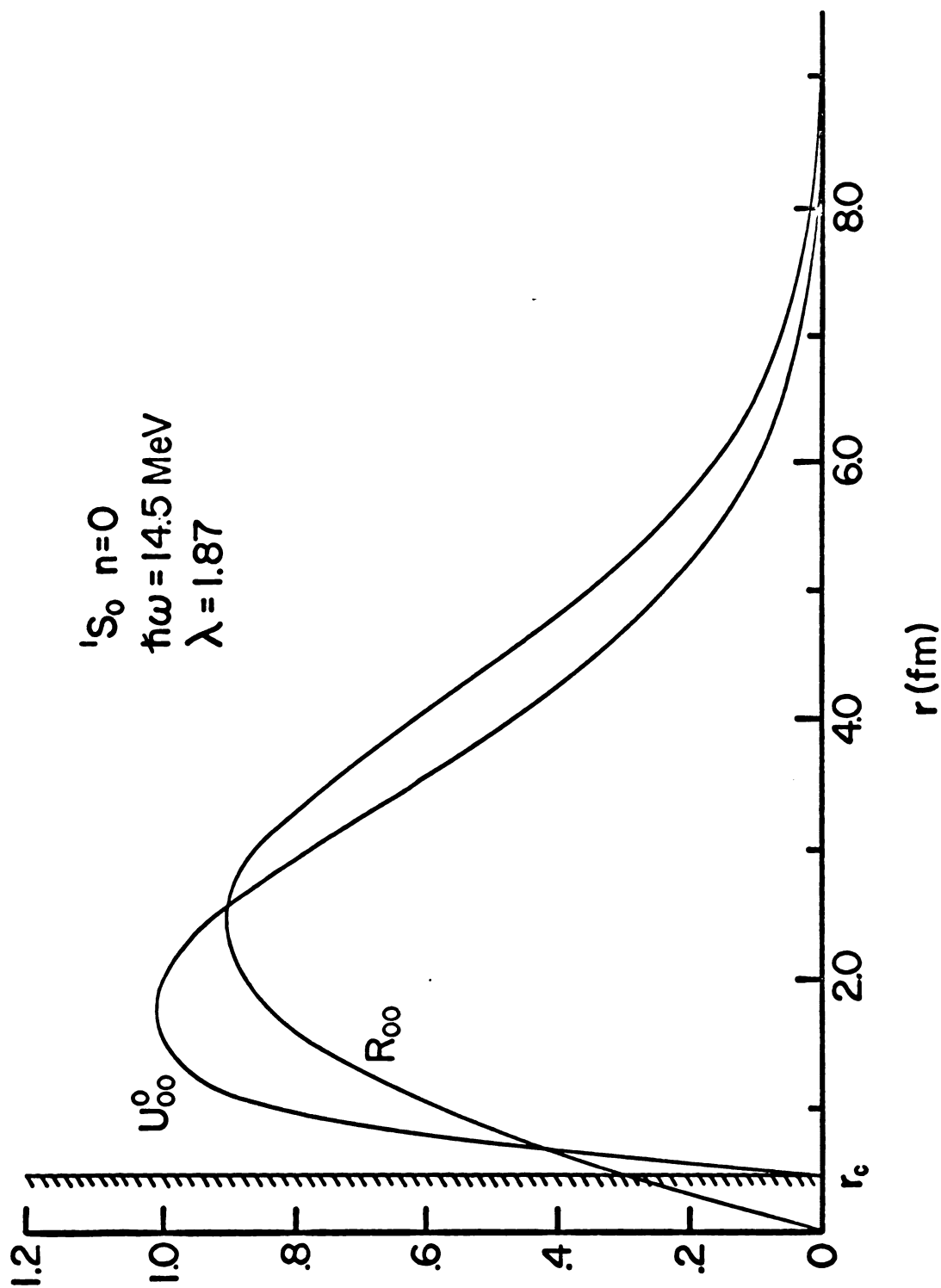


Fig. 1. --Comparison of the os solution, u_{oo}^0 , which neglects the Pauli operator with the harmonic oscillator wave function, R_{oo}^0 . λ is the eigenvalue and the Hamada-Johnston potential was used.

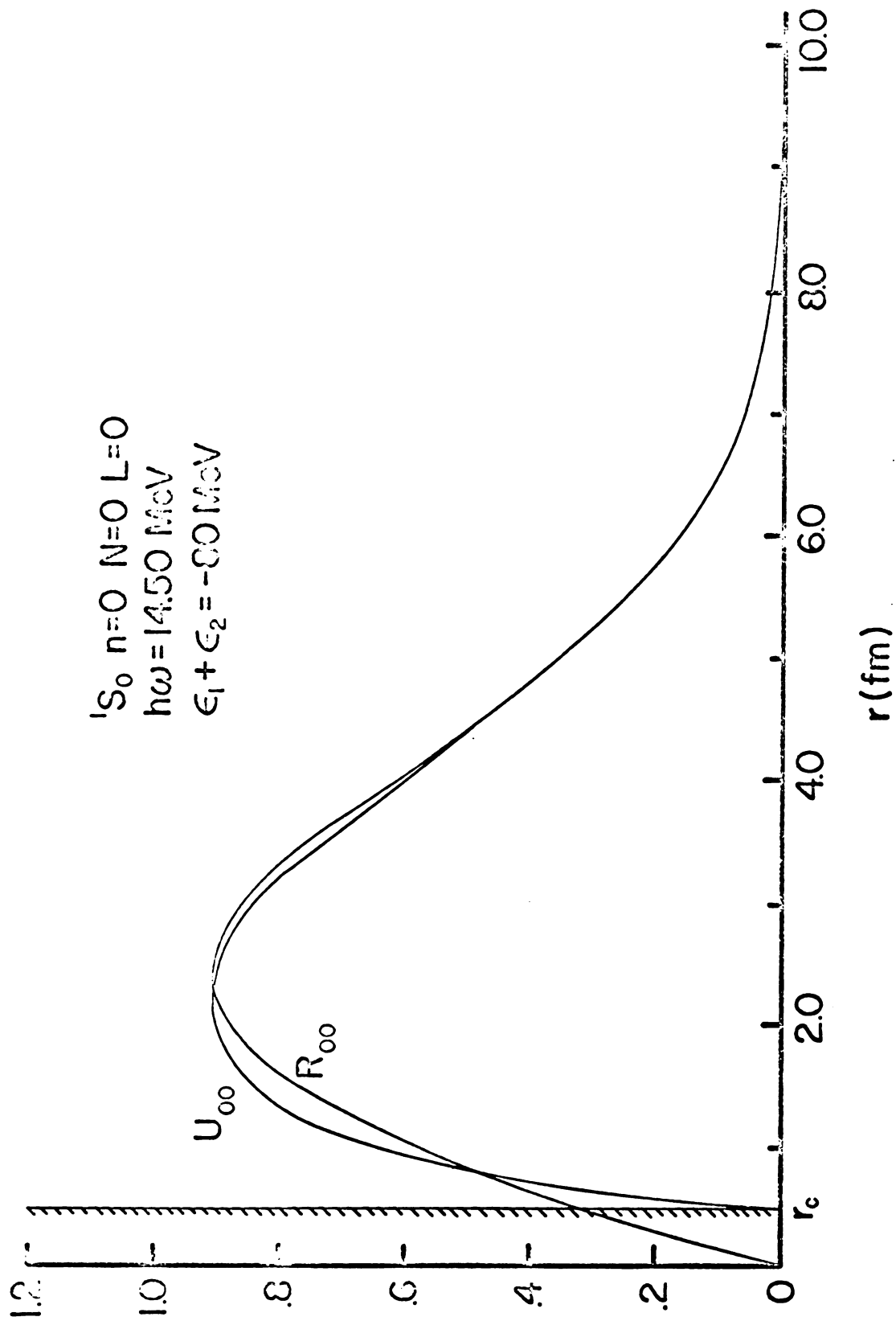


Fig. 2. --Comparison of the os Bethe-Goldstone wave function, u_{00} , with the os harmonic oscillator wave function, R_{00} . The Hamada-Johnston potential was used.

The contrast of Figures 1 and 2 explicitly displays the effect of the Pauli operator. The correct BG wave function, for all calculational purposes, has healed at 2.5 fm, and the healing is complete at 4 fm.

Similarly for the 3S_1 coupled $l = j-1$ dominate states, the solution without the Pauli operator is plotted in Figure 3 and the solution containing the Pauli operator is plotted in Figure 4. The same healing phenomenon for the dominate component of the solution occurs in the case of the coupled states at roughly the same healing distances as in the 1S_0 state. The minor component of the coupled solution is drastically reduced when the Pauli operator is included, and since the tensor force is strong, the off-diagonal tensor contribution to the matrix element $\langle \phi | \mathcal{N} | \psi \rangle$ is reduced accordingly.

The healing of the BG wave function is of fundamental significance in the nuclear many-body problem and shows precisely the effect of the Pauli operator. This phenomenon is well known and was originally investigated for the 1S_0 state in nuclear matter by Gomes, Walecka and Weisskopf.⁴ Similar results using different techniques and approximations have been reported by other authors^{9, 21} for finite nuclei. Considerable importance has

²¹H. S. Kohler and R. J. McCarthy, Nucl. Phys. 86 (1966) 611.

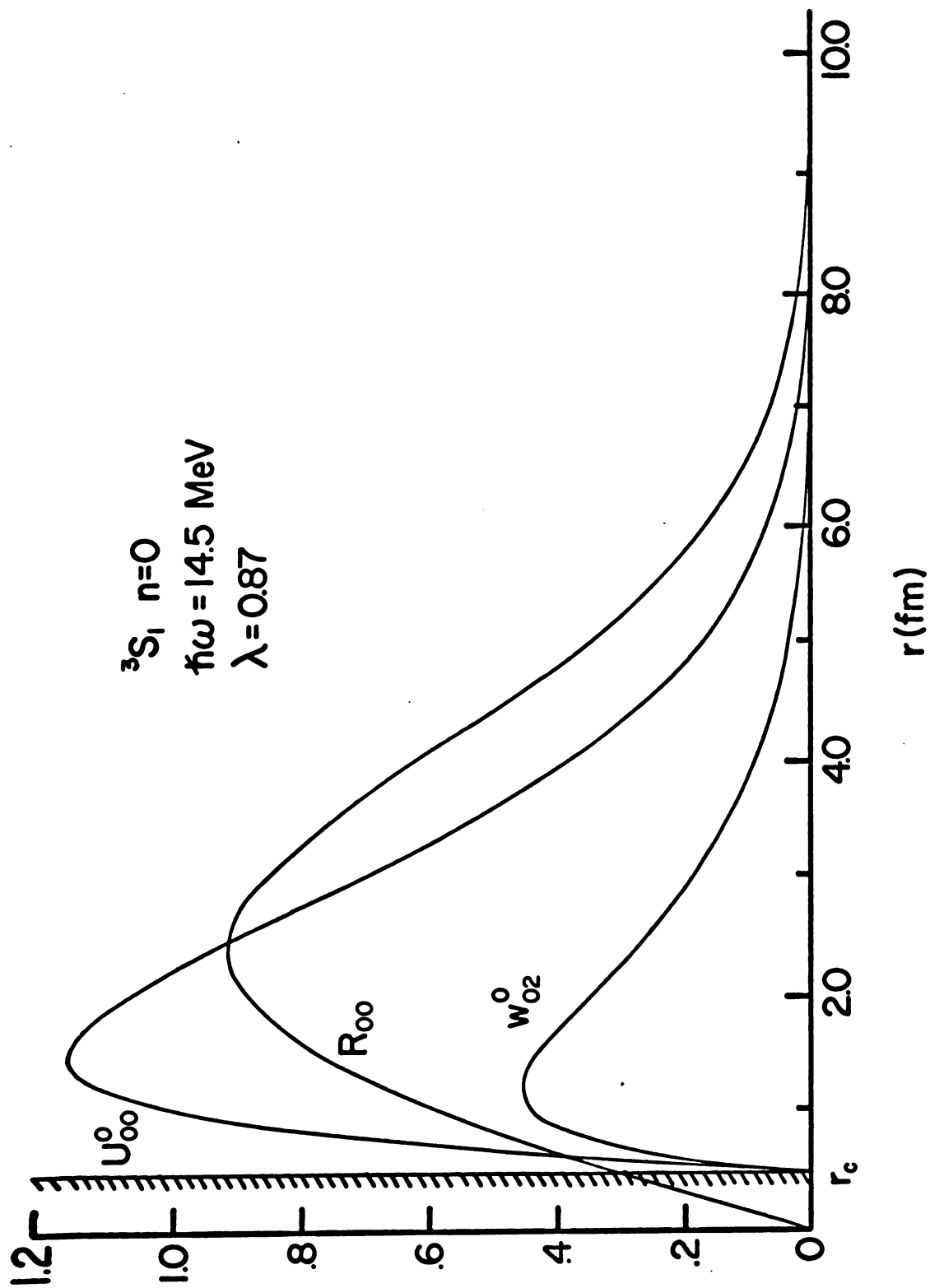


Fig. 3. --Comparison of the os triplet solution, u_{oo}^0 and w_{oo}^0 with the os harmonic oscillator wave function, R_{oo} . u_{oo}^0 is the dominant component and w_{oo}^0 is the minor component.

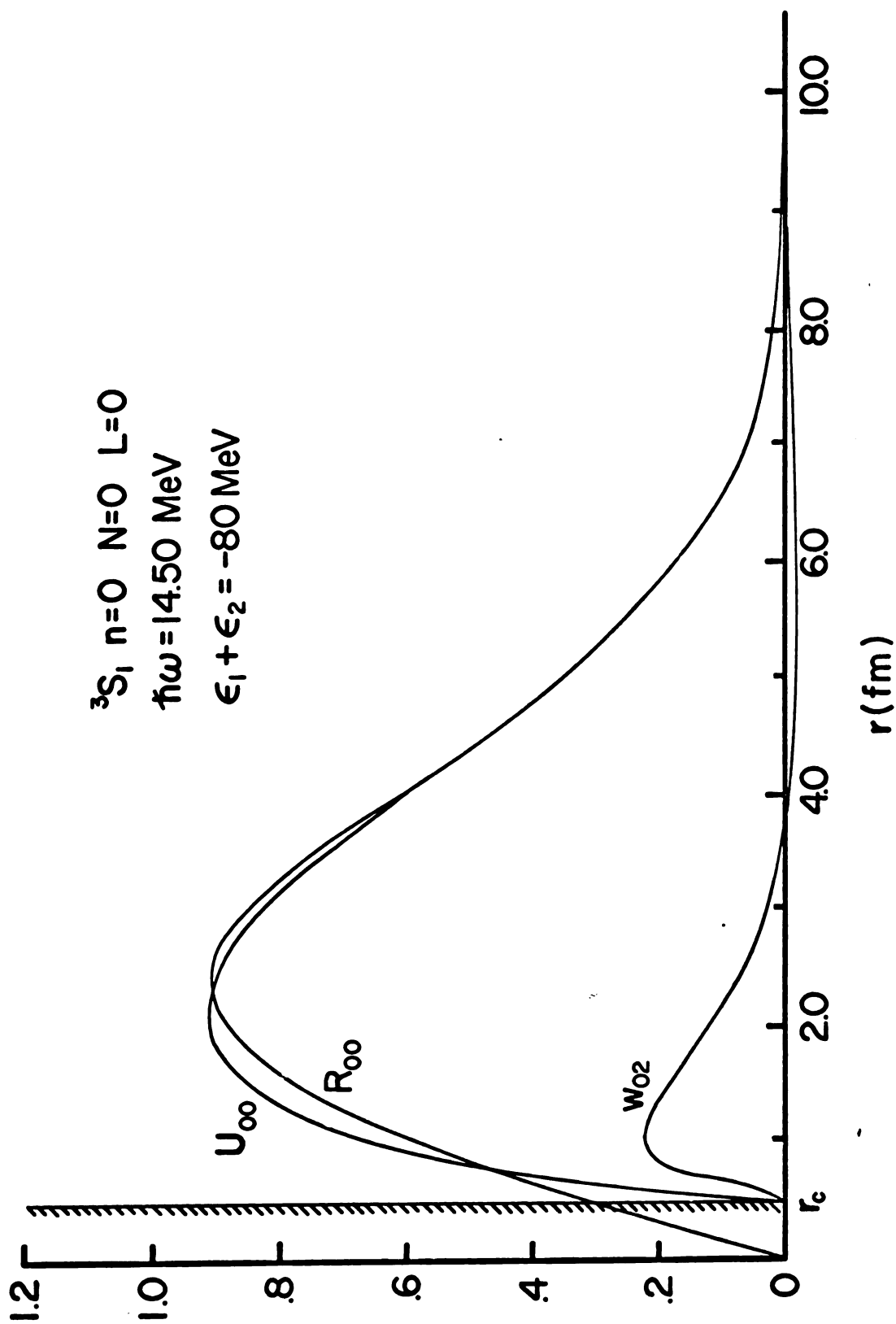


Fig. 4--Comparison of the os triplet Bethe-Goldstone wave function, u_{oo} and w_{oo2} , with the harmonic oscillator wave function, R_{oo} . u_{oo} is the dominant component and w_{oo2} is the minor component of the BG solution.

been attached to the healing property since it implies that the wave function for nucleons inside the nucleus are independent and spherically symmetric; this is precisely the assumption of the classical shell model. So the validity of the shell model comes directly from the many-body effects of the Pauli operator. Even though the aim of the many-body theory is to reproduce the experimental data and not to justify any models, it is encouraging to observe that the many-body results, in some sense, do justify the classical shell model which has had some successes in classifying nuclear data.

The healing of the BG wave function can be explained physically by viewing the interaction of the two nucleons as a scattering process in which the energy and momentum distribution of the two particles must be conserved. Since all the nearby energy states are occupied by spectator nucleons, scattering can only occur into unoccupied states. But since energy is not conserved, the particles must return to the original states with the same initial energy and momentum distribution. Hence there is no momentum transfer in the scattering process and hence the phase shift is zero. The entire process is considered to be a virtual process and the phase shifts are said to be virtual.⁶ Since there are no real phase shifts, the wave function must heal, and only at very

short distances ($r < 2\text{fm}$) can be perturbed and unperturbed wave functions be different.

In the past (references 7 and 12) healing of the wave function has been viewed as a calculational tool. That is, healing has been imposed as an additional boundary condition and considerably reduced the computation involved. The point of view of the present paper is that healing is a test of the validity of the solutions. Moreover, it is believed that the numerical techniques of Appendix B are more efficient than those using the separation method, i. e., the method which imposes healing from the beginning, and it is unnecessary to artificially force healing.

The quantitative effect of the Pauli operator can be demonstrated by comparing the diagonal t-matrices calculated with and without the Pauli operator. This has been done for several states and is shown in Table I. As can be seen from this table the effect

TABLE I. --Comparison of diagonal t-matrices (in MeV) with and without the Pauli operator using the HJ potential.

	1S_0	3S_1	1P_1	3P_0	3P_1	3P_2
Without Pauli operator	-8.2	-15.9	1.7	-2.0	1.9	-1.2
With Pauli operator	-6.4	-7.0	2.0	-2.4	2.1	-1.0

of the Pauli operator is quite large in the 3S_1 state and less important for all the other states.

In the past there has been uncertainty concerning the dependence of the BG wave function on the center-of-mass quantum numbers and the initial state HF single particle energies. The results of this study show that for the singlet and triplet $l = j$ states the center-of-mass and energy dependence are not crucial. In fact the final t-matrix results for the $l = j$ states are extremely insensitive to variations in both of these quantities. Figure 5 compares two wave functions with comparable energies and different center-of-mass quantum numbers. The differences in the two wave functions are minimal. Since the center-of-mass quantum numbers determine the number of terms which are included in the summation in equation 12 Chapter II, it has been concluded that by far the most important term in the BG equation is the term $(\lambda - \lambda^0)\phi\langle\phi|\psi\rangle$. The additional terms which enter the complicated summation contribute at most .5 MeV to the t-matrix.

The energy dependence of the 1S_0 wave function is shown in Figure 6 which compares two wave functions with the same center-of-mass quantum numbers but very different energies. Again the differences in the wave functions are slight. In order to reinforce this point the t-matrix for the 1S_0 , $N = 0$, $L = 0$ state was

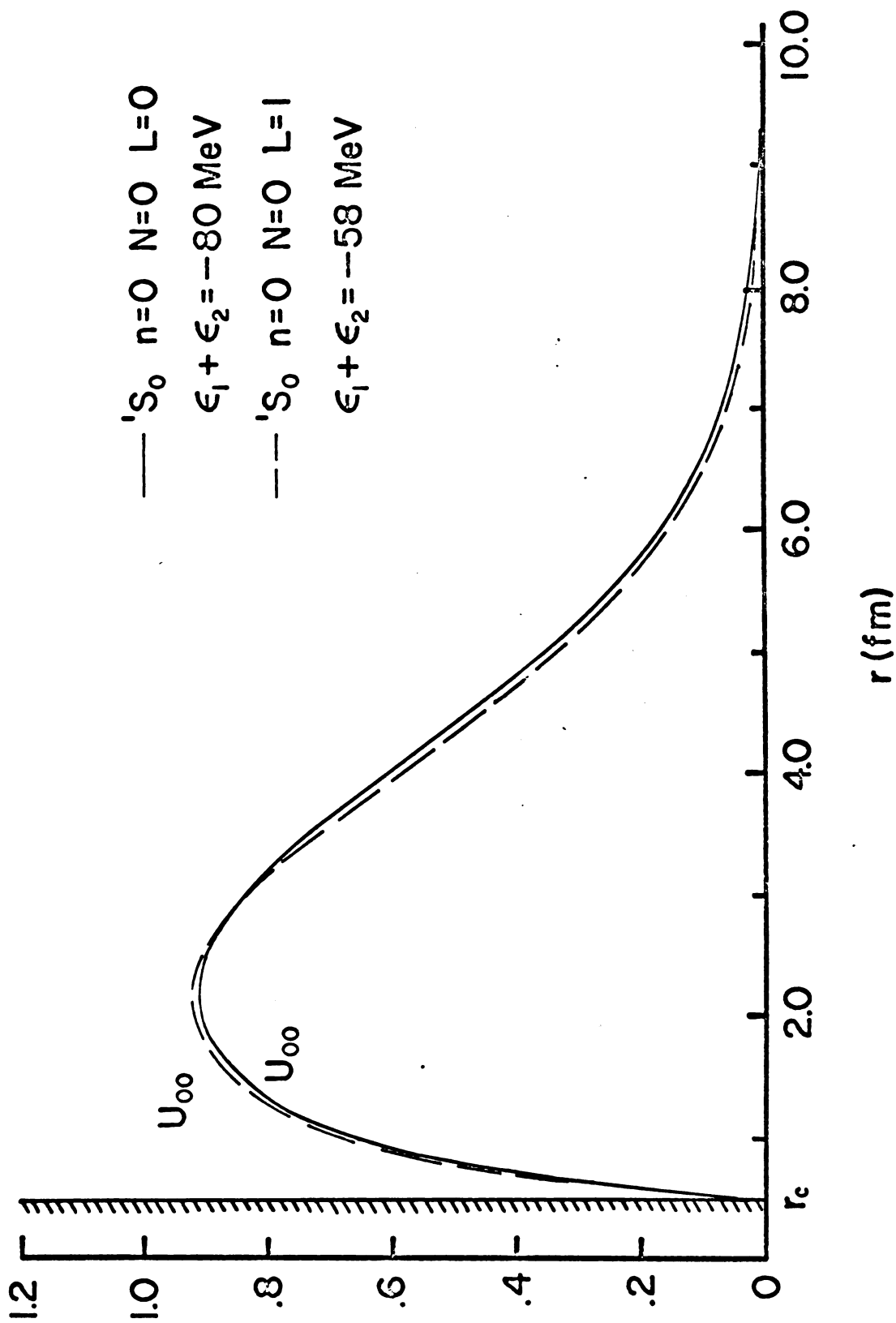


Fig. 5. --Comparison of two os singlet Bethe-Goldstone wave functions with different center-of-mass quantum numbers and slightly different singlet particle energies.

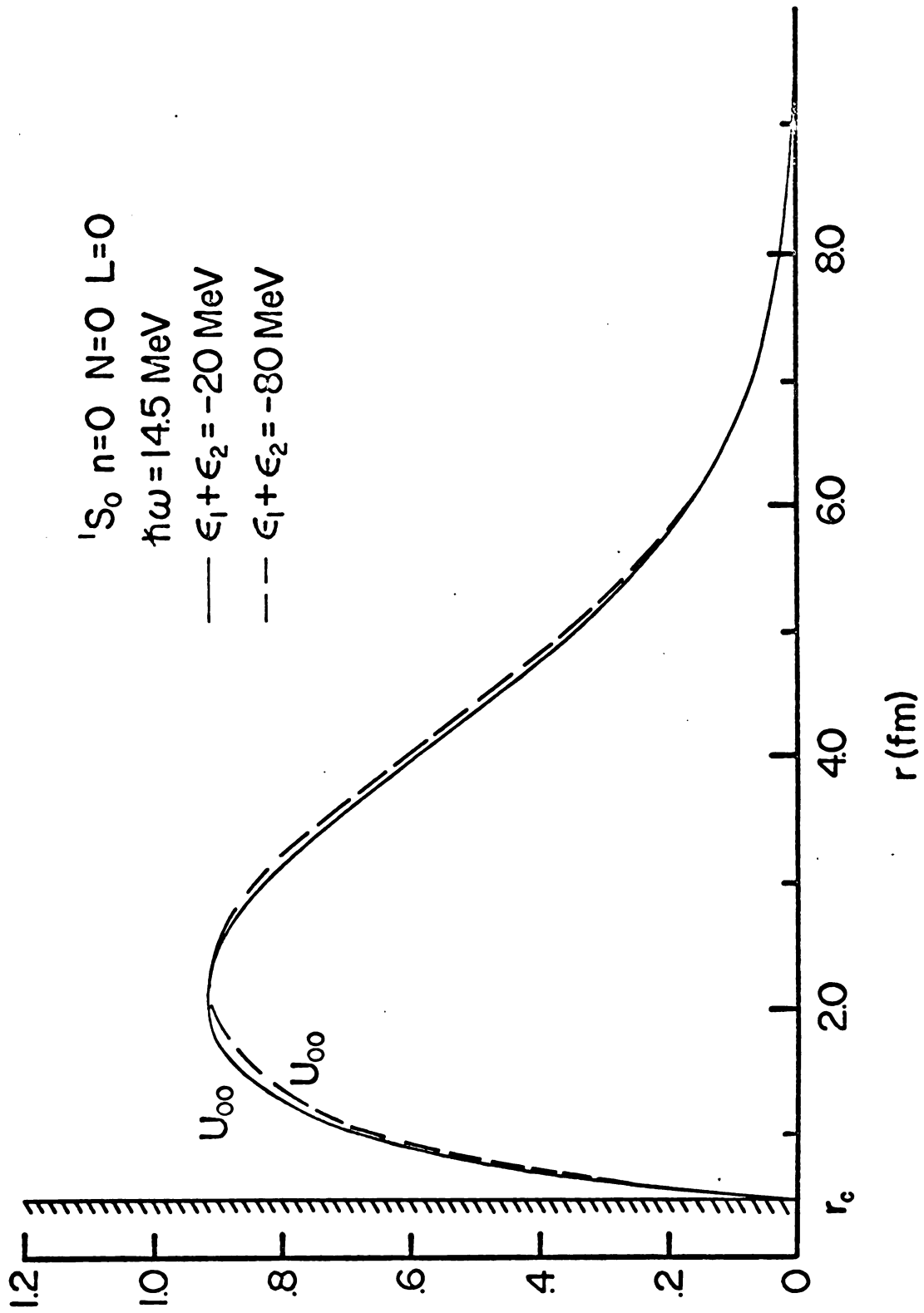


Fig. 6. --Comparison of two 1S_0 singlet Bethe-Goldstone wave functions with very different single particle energies.

calculated over a wide range of energy values and the diagonal matrix elements are plotted in Figure 7. This graph explicitly shows the insensitivity of the t-matrix to variations in the single particle energies. The final results vary less than 3% over the energy range -80 to -35 MeV which is the region of interest in ^{16}O .

For the $^3\text{S}_1$ states the results are sensitive to the energy and insensitive to the center-of-mass quantum numbers. Figure 8 shows two $^3\text{S}_1$ wave functions plotted for different values of the single particle energies. The minor component of the solution changed appreciably for different energies and this is reflected in the t-matrix through the off-diagonal element. Therefore, it is imperative that the correct choice for the energies be made in the $^3\text{S}_1$ states. Figure 9 shows that the final results vary by about 20% over the energy range -80 to -35 MeV.

The mathematical reason for the insensitivity to $\epsilon_1 + \epsilon_2$ of the $^1\text{S}_0$ state is directly related to the healing property of the wave function. In the BG equation the energy enters as a factor multiplying $(u - R)$, and since the wave function, u , approaches the unperturbed wave function, R , the term $\lambda(u - R)$ is a small quantity when compared to other terms in the integro-differential equation. The overall effect is that the BG wave function and the t-matrix are extremely independent of the energy.

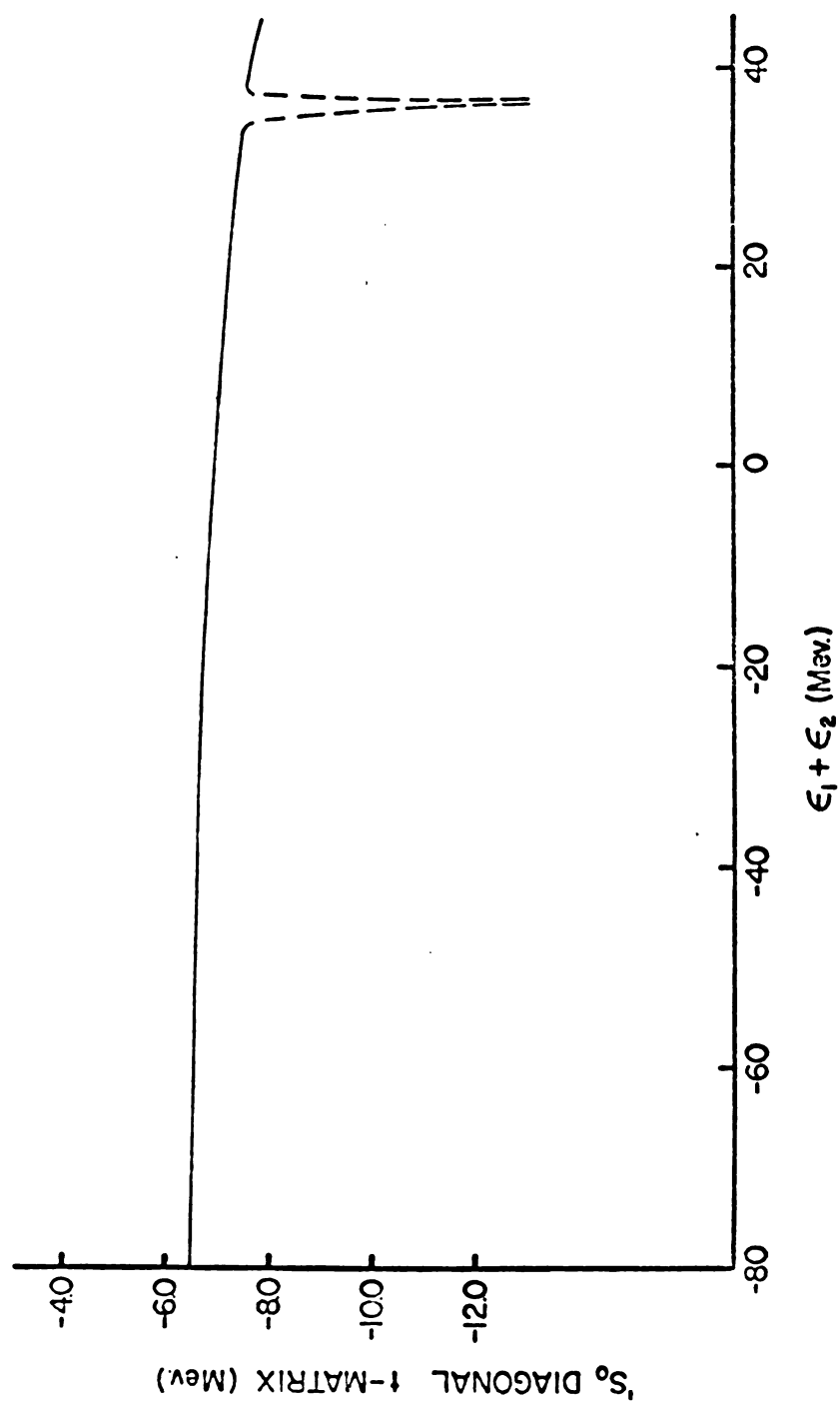


Fig. 7. --Dependence of the singlet $l=j$ reaction matrix on the Hartree-Fock single particle energies.

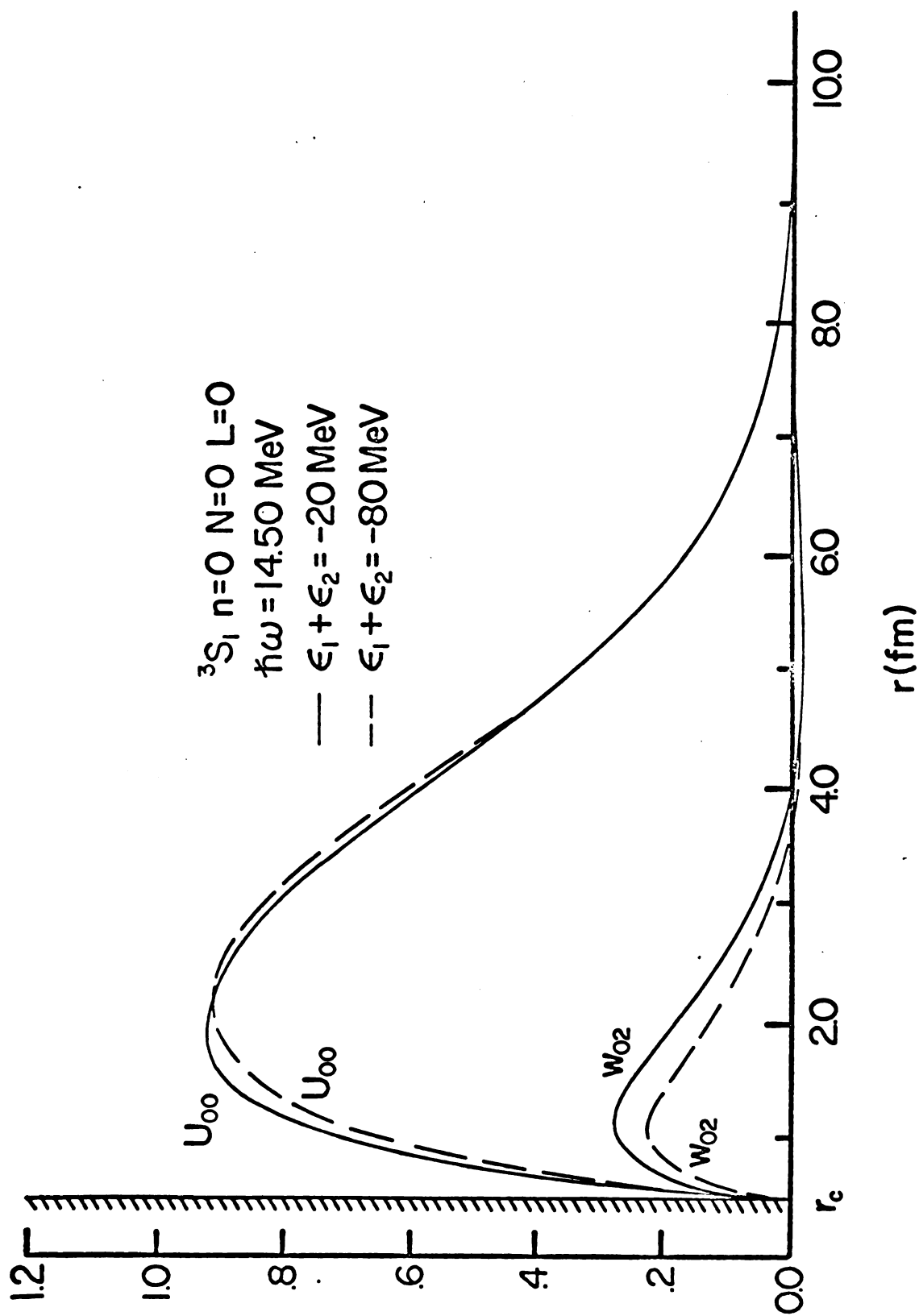


Fig. 8. -- Comparison of two 3S_1 triplet Bethe-Goldstone wave functions with very different energies. u_{00} and w_{02} are the major and minor components of the BG wave function respectively.

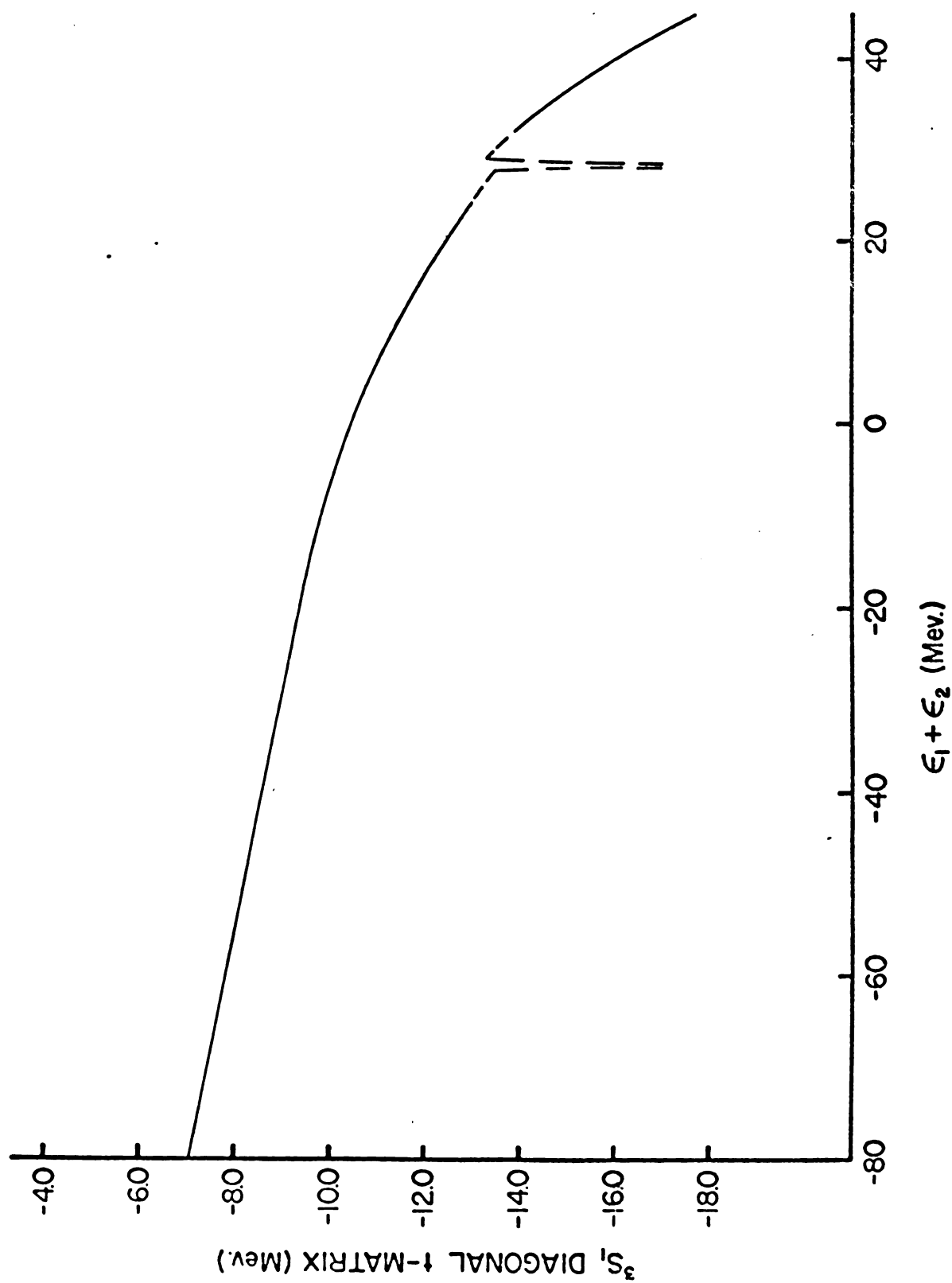


Fig. 9. --Dependence of the triplet $l=j=1$ reaction matrix on the Hartree-Fock single particle energies.

In the case of the 3S_1 state the $l = j-1$ dominant component of the solution behaves in a manner identical to the uncoupled solution. However, the $l' = j + 1$ minor component does not heal to any unperturbed solution. The resultant effect is that the minor component of the solution is sensitive to the sum of the single particle energies.

Although it was not the purpose of this investigation to study the singularities of the t-matrix, it is worth noting that they constantly occurred in all states whenever the energy was varied. Fortunately these singularities did not occur in the energy regions which are important for the calculation of the ground state energy. Theoretical investigations of these singularities have been performed in several papers ^{22, 23}, but to the author's knowledge they have never been encountered in numerical solutions of the BG equation. The fact that they do exist is evident from a cursory examination of the form of the defining equation for the t-matrix, viz., equation (1) Chapter I. The singularities shown in Figures 7 and 9

²²J. S. R. Chishold and E. J. Squires, Nucl. Phys. 13 (1959) 156.

²³V. J. Emery, Nucl. Phys. 12 (1959) 69; 19 (1960) 154.

occur roughly at those values of E which satisfy the eigenvalue equation

$$(E - H_0 - \mathcal{N}) \psi^0 = 0$$

This is not the only value of E which gives rise to singularities. They occur quite frequently for energies at and above the Fermi surface, i. e., when $\epsilon_i + \epsilon_j > 0$. Since these are of considerable theoretical interest a possible future detailed examination of them is being considered.

In the past there has never been a clear demonstration of the variation of the t -matrix from one nucleus to the next. In order to study this effect the t -matrix was calculated using a Pauli operator which is appropriate to ^{40}Ca while the single particle energies and oscillator parameter, $\hbar\omega$, were those appropriate to ^{16}O . The ^{40}Ca exclusion principle can easily be incorporated by extending the summation through the 1sod major shell in the BG equation. In Table II the results of this calculation are compared to the ^{16}O results. From this Table it is seen that there is some slight effect of the Pauli operator in going from one closed-shell nucleus to the next. All of the intermediate 1sod shell nuclei should possess Pauli operators in between the extremes of ^{16}O and ^{40}Ca . However, since the effect due to different 1sod shell Pauli

TABLE II. --The first column gives the matrix elements $\langle n'l' | t_{jS}(NL) | nl \rangle$ for ^{16}O . The last column gives the value of the reaction matrix using a Pauli operator appropriate to ^{40}Ca while the single particle energies are those of ^{16}O . The numbers in the last column are not realistic matrix elements and are listed only to display the effect of the Pauli operator in going from one major shell to another.

$\epsilon_1 + \epsilon_2$	$n'l'$	nl	jS	NL	^{16}O $\hbar\omega = 14.50$	^{40}Ca 14.50
-80	00	00	00	00	-6.445	-6.342
	10				-4.897	-4.811
	00	00	11	00	-7.051	-6.646
	10				-5.206	-4.945
	02				-6.373	-6.364
	12				-8.939	-8.873
-58	00	00	00	01	-6.572	-6.467
	10				-5.011	-4.924
	00	00	11	01	-7.519	-7.228
	10				-5.571	-5.389
	02				-6.403	-6.367
	12				-9.035	-8.928
-36	00	00	00	02 (10)	-6.616	-6.575
	10				-5.057	-5.023
	00	00	11	02 (10)	-7.774	-7.637

TABLE II. --continued

$\epsilon_1 + \epsilon_2$	n'l'	nl	jS	NL	^{16}O	^{40}Ca
					$\hbar\omega = 14.50$	14.50
	10				-5.808	-5.724
	02				-6.407	-6.396
	12				-9.051	-9.012
	00	10	00	00	-5.278	-5.241
	10				-4.451	-4.420
	00	10	11	00	-6.767	-6.489
	10				-5.576	-5.396
	02				-3.102	-3.124
	12				-6.117	-6.125

operators is slight, it would be adequate to use some interpolated values for these nuclei since a precise calculation for these nuclei is extremely difficult, if not impossible.

Solutions for a few of the higher angular momentum and higher nodal states are shown in Figures 10, 11, 12, and 13. In general these solutions exhibit the same properties as the previously discussed solutions. The higher angular momentum states heal more rapidly than the S-states and are almost completely independent of the values of the single particle energies.

Bethe et al.¹¹ have shown that the t-matrix should be Hermitian. The Hermiticity was tested for only the 1S_0 and 3S_1 states. By actual calculation with the same particle energies for the relative 1s and 0s states, the following results were obtained:

$$\langle 10 | t_{00}(00) | 00 \rangle = -4.89 \qquad \langle 00 | t_{00}(00) | 10 \rangle = -4.81$$

and

$$\langle 10 | t_{11}(00) | 00 \rangle = -5.21 \qquad \langle 00 | t_{11}(00) | 10 \rangle = -5.41$$

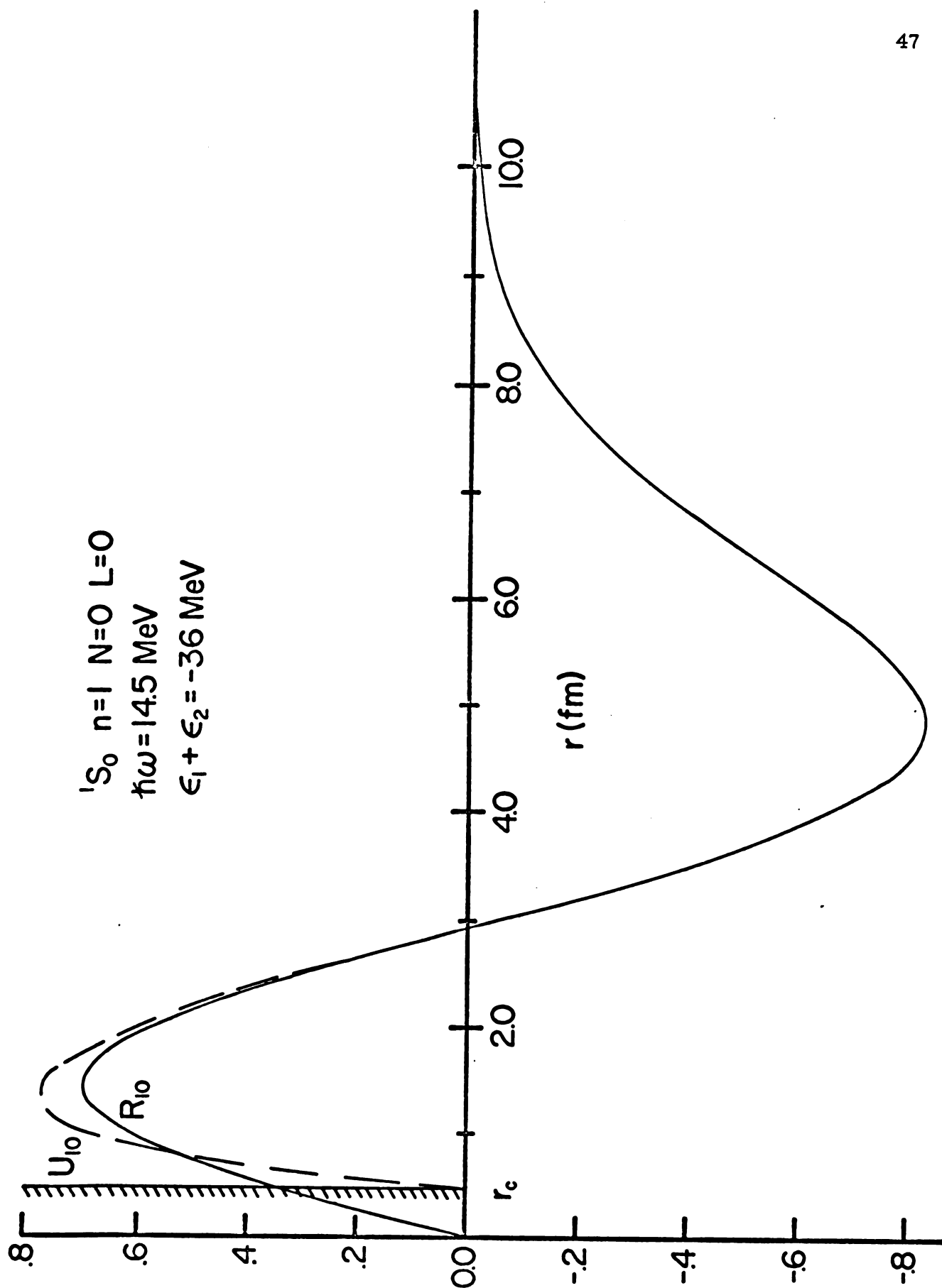


Fig. 10. --Comparison of the 1s Bethe-Goldstone wave function, u_{10} , with the 1s harmonic oscillator wave function, R_{10} . The healing is more rapid than for the os solution.

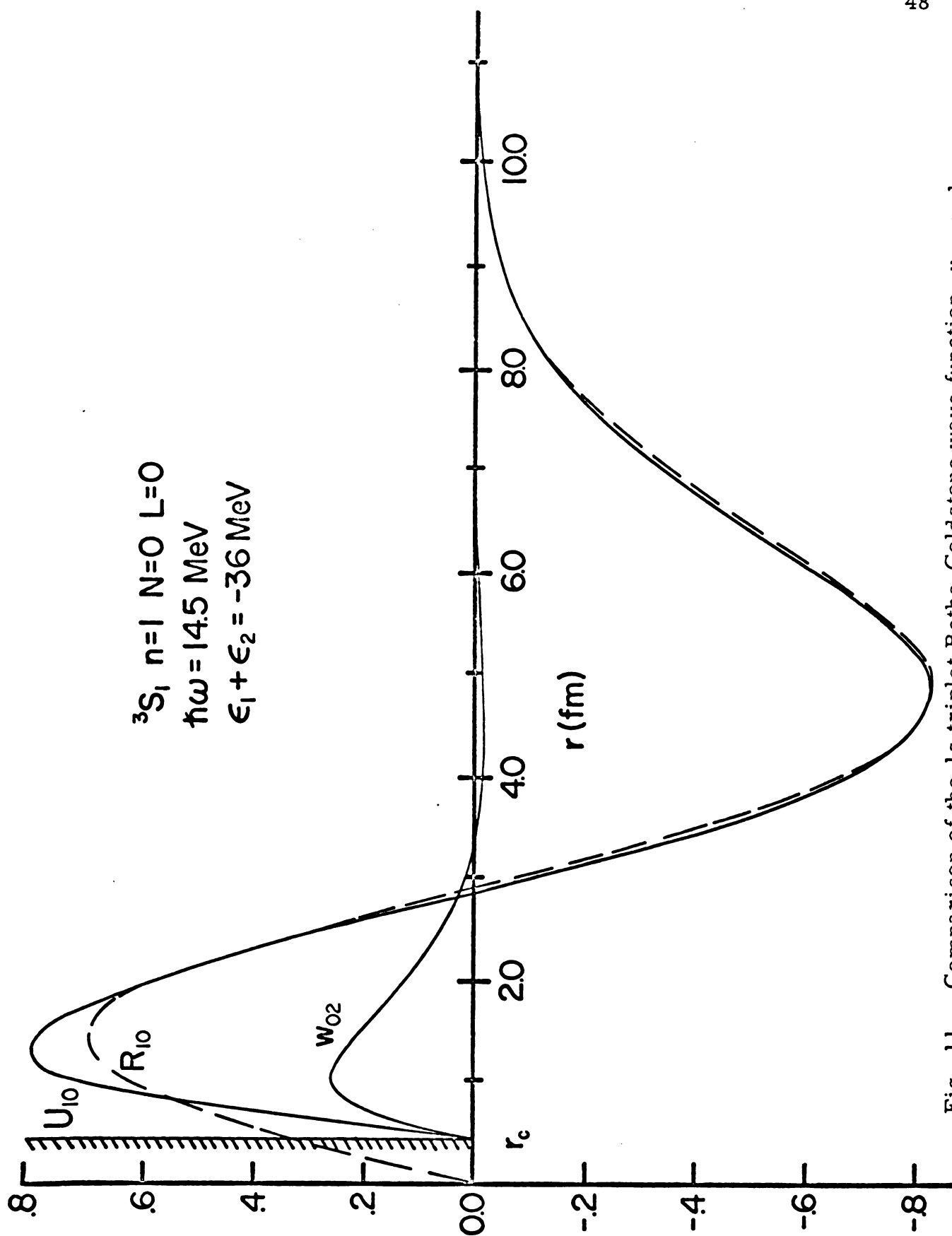


Fig. 11. --Comparison of the 1s triplet Bethe-Goldstone wave function, u_{10} and w_{02} , with the harmonic oscillator wave function, R_{10} . u_{10} and w_{02} are the major and minor components of the solution respectively.

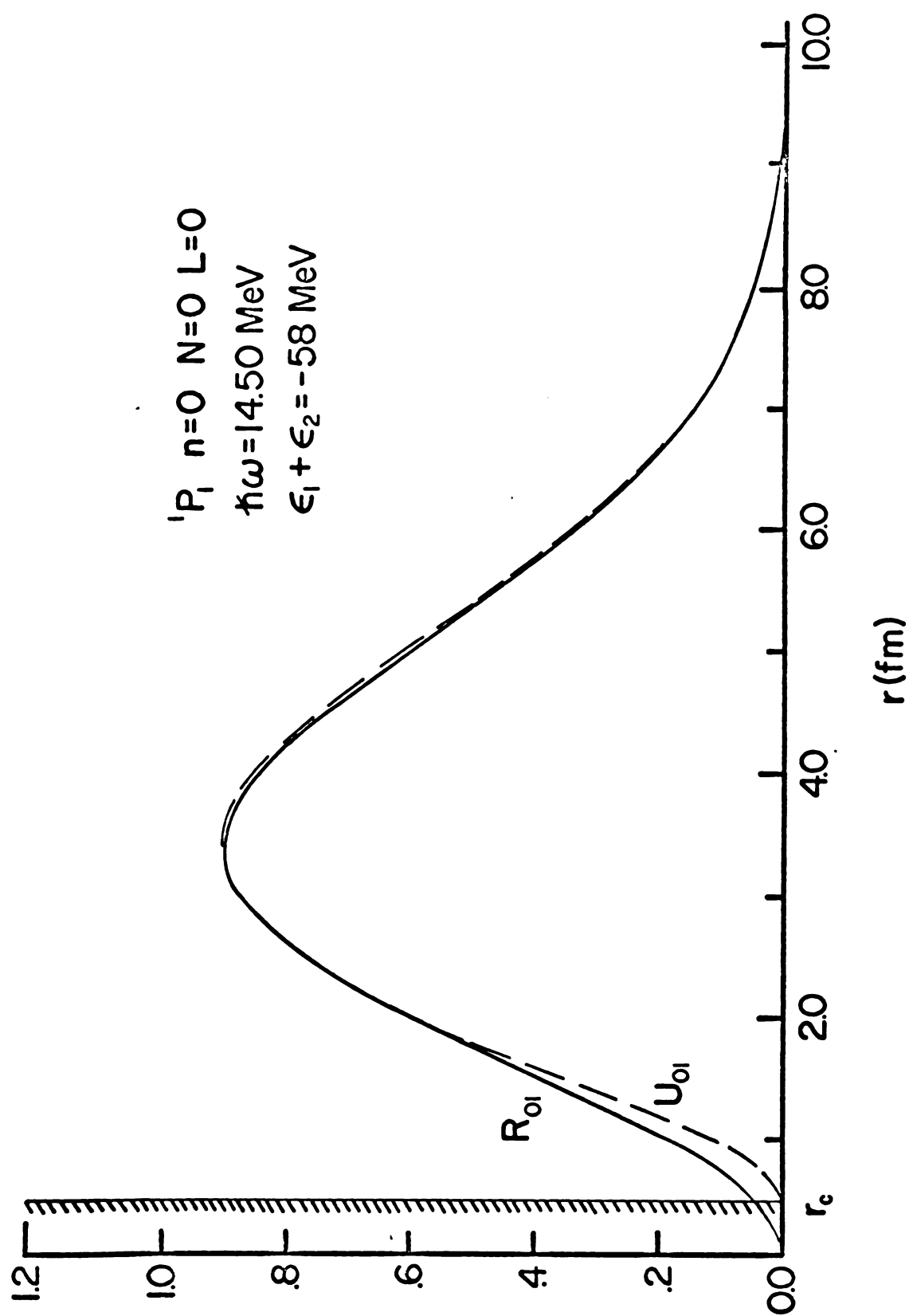


Fig. 12. --Comparison of the op Bethe-Goldstone wave function, u_{01} , with the harmonic oscillator wave function, R_{01} . The wave function heals more rapidly than in any of the S-states.

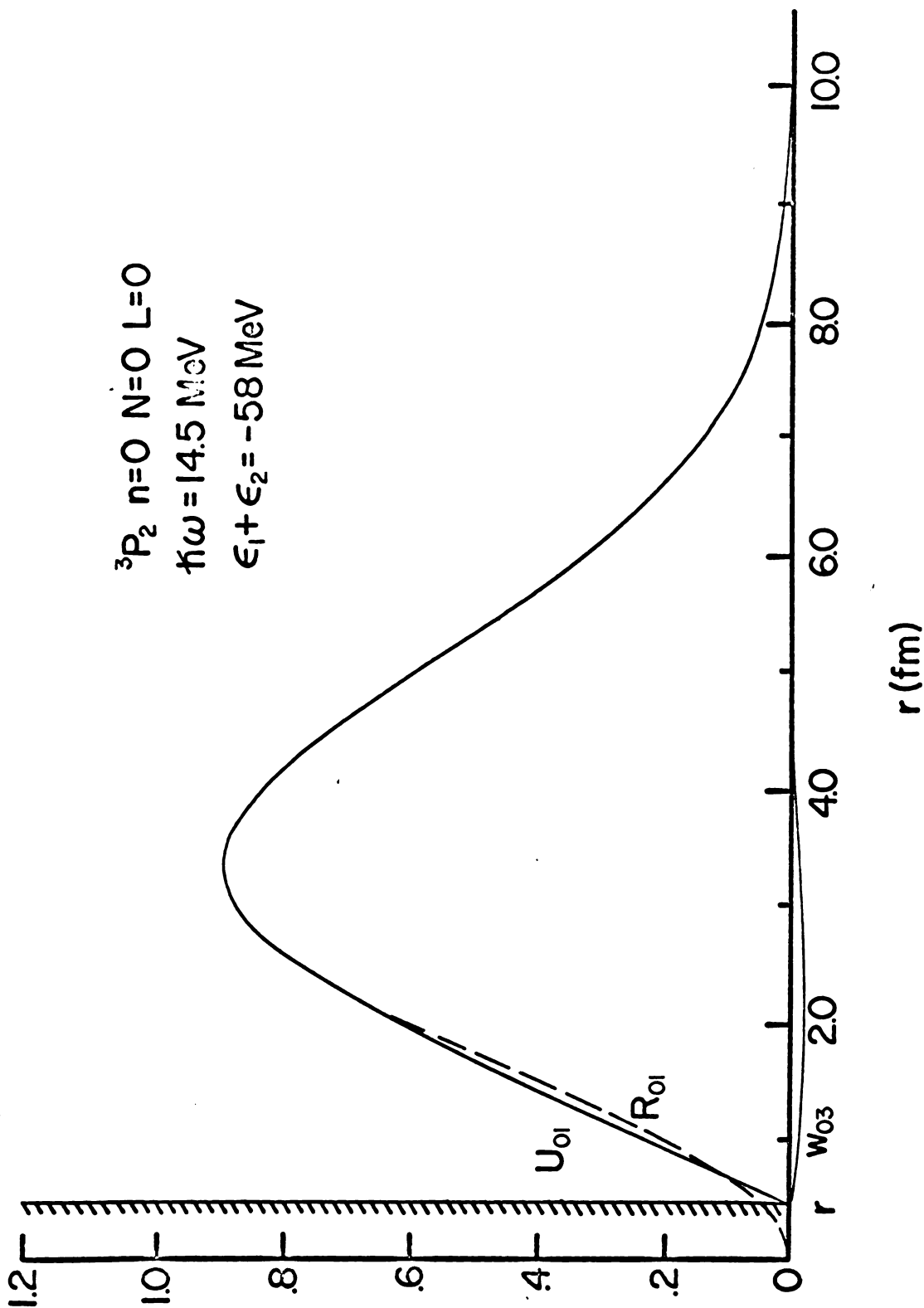


Fig. 13. --Comparison of the op triplet Bethe-Goldstone wave function with the harmonic oscillator wave function, R_{01} . The minor component w_{03} is almost negligible and the healing is quite rapid.

where the notation is

$$\langle n'l' | t_{js}^{(NL)} | nl \rangle$$

A complete list of the t-matrices relevant for the ground state properties of ^{16}O are listed for the HJ and BGT potentials in Tables III and IV respectively. The single particle energies, -80, -58 and -36 MeV, correspond to the two particles in the osos, osop, and opop states respectively. These values are the results which were ultimately used in calculating the binding energies.

Once a good set of t-matrix elements has been obtained there exists a wealth of experimental data which should provide good tests for both the t-matrix and the numerical results. Unfortunately rigorous tests usually involve either shell-model or Hartree-Fock calculations. Each of these calculations involves considerable effort. However, it is possible to immediately calculate the approximate binding energy of ^{16}O and the $\overline{1}\cdot\overline{5}$ splitting in ^{17}O .

In Appendix D it was shown that the approximate binding energy of ^{16}O is given by the following

TABLE III.--Matrix elements, $\langle n'l' | t_{jS}(\text{NL}) | nl \rangle$, for HJ potential.

$\epsilon_1 + \epsilon_2$	$n'l'$	nl	jS	NL	$\hbar\omega$		
					13.35	14.50	15.50
-80	00	00	00	00	-5.973	-6.445	-6.838
	10				-4.733	-4.897	-4.988
	00	00	11	00	-6.617	-7.051	-7.397
	10				-5.127	-5.206	-5.222
	02				-5.578	-6.373	-7.089
	12				-7.892	-8.939	-9.873
-58	00	00	00	01	-6.101	-6.572	-6.962
	10				-4.852	-5.011	-5.106
	00	00	11	01	-7.080	-7.519	-7.867
	10				-5.508	-5.571	-5.568
	02				-5.612	-6.403	-7.115
	12				-7.987	-9.035	-9.968
	01	01	10	00	1.757	2.029	2.284
	11				1.875	2.197	2.504
	01	01	01	00	-2.144	-2.389	-2.599
	11				-1.779	-1.902	-1.993
	01	01	11	00	1.849	2.133	2.393
	11				1.985	2.279	2.549

TABLE III.--continued

$\epsilon_1 + \epsilon_2$	n'l'	nl	jS	NL	$\hbar\omega$		
					13.35	14.50	15.50
-36	01	01	21	00	-0.834	-0.990	-1.135
	11				-1.118	-1.310	-1.485
	03				0.682	0.794	0.896
	13				+0.924	1.062	1.185
	00	00	00	02 (10)	-6.150	-6.616	-7.001
	10				-4.904	-5.057	-5.147
	00	00	11	02 (10)	-7.363	-7.774	-8.094
	10				-5.776	-5.808	-5.776
	02				-5.617	-6.407	-7.117
	12				-8.007	-9.051	-9.981
	00	10	00	00	-5.062	-5.278	-5.430
	10				-4.426	-4.451	-4.425
	00	10	11	00	-6.566	-6.767	-6.876
	10				-5.631	-5.576	-5.454
	02				-2.809	-3.102	-3.345
	12				-5.470	-6.117	-6.673
	02	02	20	00	-0.497	-0.589	-0.675
	12				-0.552	-0.650	-0.740

TABLE III. --continued

$\epsilon_1 + \epsilon_2$	n'l'	nl	jS	NL	$\hbar\omega$		
					13.35	14.50	15.50
	02	02	11	00	1.676	1.361	1.537
	12				1.099	1.252	1.389
	00				-5.571	-6.363	-7.076
	10				-2.853	-3.141	-3.386
	02	02	21	00	-2.114	-2.459	-2.772
	12				-2.141	-2.443	-2.710
	02	02	31	00	0.038	+0.044	0.049
	12				0.025	+0.026	0.027
	04				-1.039	-1.239	-1.427
	14				-1.403	-1.652	-1.882

TABLE IV. --Matrix elements, $\langle n'l' | t_{jS}(NL) | nl \rangle$, for BGT potential.

$\epsilon_1 + \epsilon_2$	$n'l'$	nl	jS	NL	$\hbar\omega$		
					13.35	14.50	15.50
-80	00	00	00	00	-6.222	-6.683	-7.061
	10				-4.697	-4.795	-4.838
	00	00	11	00	-7.817	-8.426	-8.931
	10				-6.896	-7.199	-7.416
	02				-5.603	-6.371	-7.055
	12				-7.879	-8.791	-9.608
58	00	00	00	01	-6.343	-6.800	-7.174
	10				-4.806	-4.897	-4.933
	00	00	11	01	-8.317	-8.939	-9.453
	10				-7.302	-7.594	-7.797
	02				-5.627	-6.389	-7.067
	12				-7.968	-8.881	-9.698
	01	01	10	00	2.553	2.916	3.242
	11				2.574	2.881	3.156
	01	01	01	00	-2.983	-3.302	-3.575
	11				-2.342	-2.479	-2.584
	01	01	11	00	1.992	2.288	2.558
	11				2.087	2.373	2.637
	01	01	21	00	-1.336	-1.553	-1.752

TABLE IV. --continued

$\epsilon_1 + \epsilon_2$	n'l'	nl	jS	NL	13. 35	$\hbar\omega$ 14. 50	15. 50
-36	11				-1. 584	-1. 823	-2. 041
	03				0. 930	1. 071	1. 199
	13				1. 254	1. 404	1. 542
	00	00	00	02 (10)	-6. 388	-6. 814	-7. 210
	10				-4. 853	-4. 940	-4. 917
	00	00	11	02 (10)	-8. 554	-9. 150	-9. 683
	10				-7. 519	-7. 782	-7. 459
	02				-5. 621	-6. 381	-7. 058
	12				-7. 969	-8. 879	-9. 694
	00	10	00	00	-4. 928	-5. 064	-5. 143
	10				-4. 094	-4. 038	-3. 946
	00	10	11	00	-7. 848	-8. 187	-8. 439
	10				-7. 117	-7. 214	-7. 246
	02				-2. 518	-2. 698	-2. 841
	12				-4. 921	-5. 360	-5. 749
	02	02	20	00	-0. 668	-0. 809	-0. 942
	12				-0. 862	-1. 015	-1. 159
	02	02	11	00	1. 761	2. 030	2. 313

TABLE IV. --continued

$e_1 + e_2$	n'l'	nl	jS	NL	$\hbar \omega$		
					13.35	14.50	15.50
	12				1.804	2.031	2.270
	00				-5.701	-6.367	-7.050
	10				-2.653	-2.815	-2.965
	02	02	21	00	-2.298	-2.718	-3.106
	12				-2.659	-3.060	-3.429
	02	02	31	00	0.095	0.079	0.058
	12				-0.087	-0.155	-0.269
	04				-1.088	-1.312	-1.524
	14				-1.656	-1.915	-2.161

$$B.E. = 18\hbar\omega + \frac{1}{2} \sum_{TSj} \sum_{m/NL} (2T+1)(2j+1)(1-(-1)^{l+s+T}) \langle mlsj | t(NL) | mlsj \rangle$$

$$\times \sum_{\substack{\text{OCCUPIED} \\ m_1 l_1 m_2 l_2}} \sum_{\Lambda} \frac{(2\Lambda+1)}{(2l+1)} \left| \langle m_1 l_1 m_2 l_2 | m l N L, \Lambda \rangle \right|^2$$

The coefficients in this expression have been tabulated by Mackellar⁹ and have been used in this paper to calculate the binding energy per nucleon as a function of the oscillator parameter, $\hbar\omega$. The final results are plotted in Figure 14 for the HJ and BGT potentials. For the HJ potential a minimum of -3.6 MeV/A occurs at about $\hbar\omega = 14$ MeV, and for the BGT potential a minimum of -7.8 MeV/A occurs at about $\hbar\omega = 18$ MeV. The experimental value is -7.98 MeV/A.²⁴

The BGT potential is known²⁵ to be unacceptable as a fit to nucleon-nucleon scattering for the $T = 1$ states, but is as good as the HJ for the $T = 0$, 3S_1 state. Since the central force is not affected as much as the tensor force by the Pauli operator and since the BGT triplet force has a strong central part, its 3S_1 matrix elements give much more binding than the HJ potential (see TABLES III and IV).

²⁴L. A. Konig, J. H. Mattauch, and A. H. Wapstra, Nucl. Phys. 31 (1962) 18.

²⁵P. Signell and N. R. Yoder, Phys. Rev. 132 (1963) 1707.

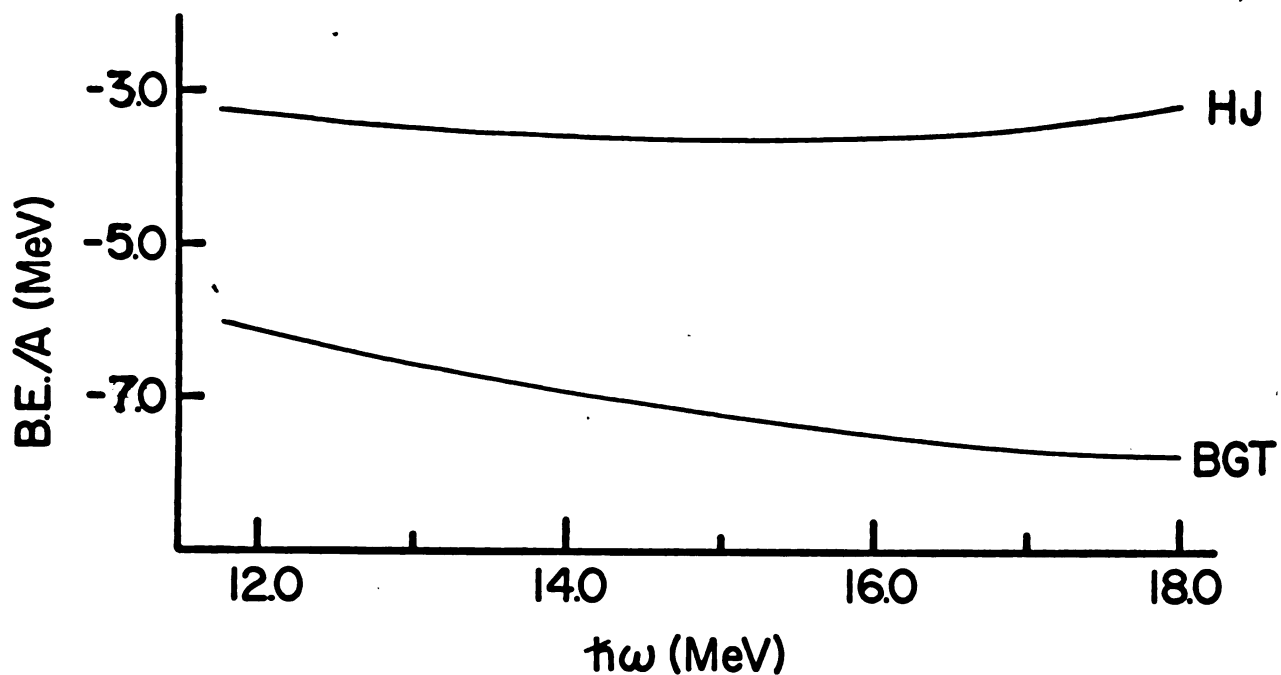


Fig. 14. --The binding energy per nucleon for ^{16}O as a function of the oscillator parameter for the Hamada-Johnston and Brueckner-Gammel-Thaler potentials.

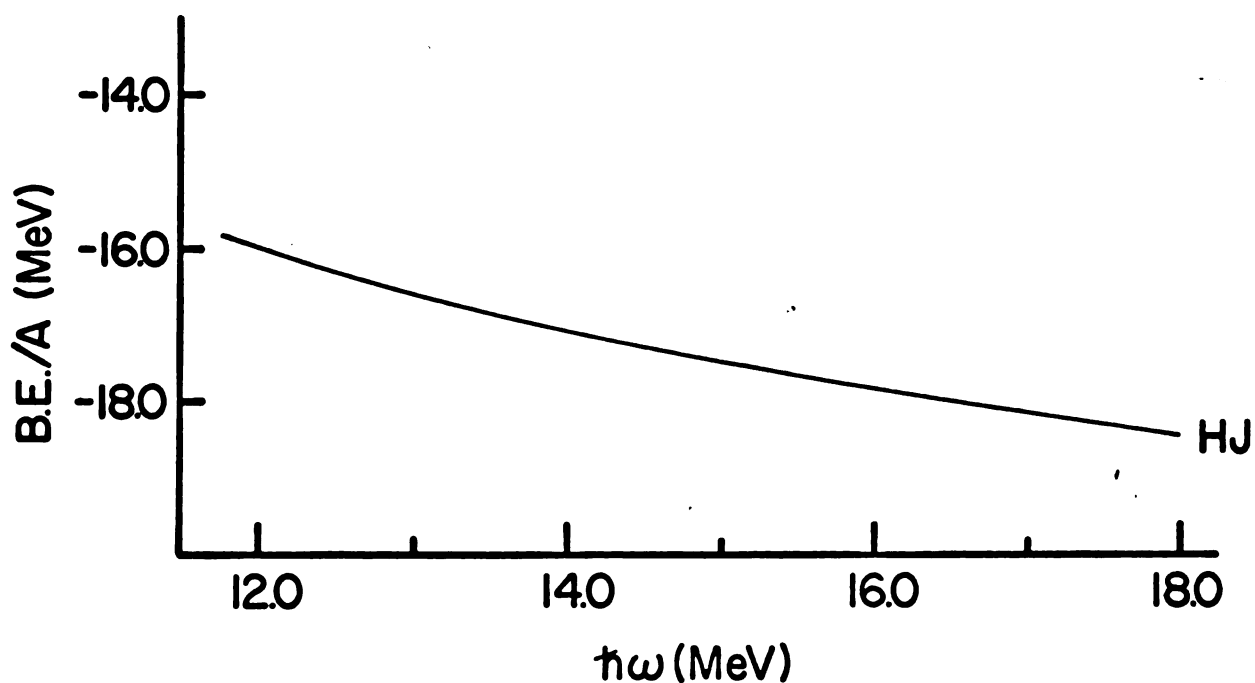


Fig. 15. --The binding energy per nucleon for ^{16}O when the Pauli operator is neglected.

Moreover, it appears that the calculations of binding energies in finite nuclei will follow the oscillating path of nuclear matter calculations.²⁶ Clearly higher order effects need to be examined for finite nuclei as they have been for nuclear matter.

A series of papers^{7, 8, 9, 26} on binding energy calculations for ^{16}O by different authors using different methods reveal considerable discrepancies. Table V is a sample listing of the t-matrix and B. E. /A results of different authors.

TABLE V. --Comparison of diagonal t-matrix, $\langle nl | t_{jS}(\text{NL}) | nl \rangle$, and B. E. /A with results of various authors using the HJ potential.

	Kuo & Brown	Wong	MacKellar	Kohler & McCarthy	Present Calculation
$\hbar\omega$	14.0	13.5	20.7	10.5	14.5
$\langle 00 t_{01}(00) 00 \rangle$	-5.61	-5.7	-9.57	-4.36	-6.44
$\langle 00 t_{13}(00) 00 \rangle$	-9.73	-6.2	-11.22	-5.37	-7.05
B. E. /A	-5.5	--	-8.0	-2.70	-3.6

²⁶S. A. Moszkowski, Rev. Mod. Phys. 39 (1967) 657.

Although the results of Mackellar fit the experimental B. E. / A quite well there is considerable doubt about the Eden-Emery treatment of the intermediate single particle energies. Moreover, the value of $\hbar\omega$ at which self-consistency is obtained is about 20 MeV and this seems at variance with the experimentally determined value of 14 MeV.²⁰ As suggested by Kohler and McCarthy²⁷ it would be of interest to see the Eden-Emery calculations repeated treating the energy denominators in a more precise manner.

It is interesting to observe that the calculations of Wong,⁸ Kuo and Brown,⁷ and Kohler and McCarthy²⁷ are similar to the results of this paper. This is somewhat remarkable since their calculations are quite different in both point of view and in calculational details. In particular the choice of the intermediate state energies in those papers are the free particle energies as opposed to harmonic oscillator energies used in this paper.

It is difficult to compare the present calculation with that of Kallio and Day²⁸ since they choose a potential which is radically

²⁷H. S. Kohler and R. J. McCarthy, Nucl. Phys. 99 (1967) 65.

²⁸A. Kallio and B. D. Day, Phys. Letters, 25 (1967) 72.

different from the HJ potential and ignores the difficulties of the tensor force.

It is interesting to compare the B. E. /A calculated with and without the Pauli operator. Figure 15 is a plot of the binding energy per nucleon calculated without the Pauli operator. There is no minimum as there is when the Pauli operator is included and the nucleons are greatly overbound by about 8 MeV/A.

As a final calculation the $\bar{T} \cdot \bar{S}$ splitting in ^{17}O was computed using an approximate expression due to Nigam:²⁹

$$E_{j=5/2} - E_{j=3/2} = \frac{1}{16} [90 V_{01}^{TS} + 55 V_{02}^{TS} + 161 V_{03}^{TS} + 9 V_{11}^{TS}]$$

where

$$V_{nl}^{TS} = \langle nl | V^{TS} | nl \rangle$$

and

$$V^{TS} = V^{TS}(r) \bar{T} \cdot \bar{S}$$

The experimentally observed splitting is 5.9 MeV and the calculated results are 4.01 and 4.56 MeV using the HJ and BGT potentials respectively.

²⁹B. P. Nigam, to be published

CHAPTER IV

CONCLUSION

The results of this study show that it is possible to solve the Bethe-Goldstone equation exactly for finite nuclei. The Pauli operator for finite nuclei has been treated in an exact manner and its qualitative and quantitative effects have been examined in detail. It has been found that when the Pauli operator is treated correctly the BG wave function heals properly to the unperturbed wave function. In addition it has been shown that the effect of the Pauli operator on the t-matrix is appreciable in the 3S_1 states and moderate in all other states. Since the numerical methods developed to solve the BG equation with the exact Pauli operator are so efficient it seems unwarranted in future calculations to make various questionable approximations when solving the BG equation. With accurate two body t-matrices available it is now possible to examine the higher order effects with more confidence.

Since the current trend in nuclear structure calculations for both the ground state and excited state properties^{3, 30, 31} relies

³⁰S. Das Gupta & M. Harvey, Nucl. Phys. A94 (1967) 602

³¹Ripka, Lectures in Theoretical Physics Vol. VIII B (1965) 237

upon HF calculations an examination of the t-matrix dependence on the HF single particle energies was performed. It was concluded that the t-matrix for the 3S_1 state is sensitive to the single particle spectrum, and in doing a HF calculation it is important that these single particle energies be chosen correctly. For other states the single particle energies are not critical, and it should not be necessary to treat these in a self-consistent manner.

The calculation of the binding energy per nucleon in this study and in those of references 7, 8, and 27 using the HJ potential give 2.7 to 5.5 MeV as compared to the observed value of 7.98 MeV. Kuo and Lynch³² report similar results using the Yale and Reid potentials. These discrepancies clearly show that it will be necessary to perform additional calculations, and there are several improvements in these calculations which need to be incorporated.

The first possible improvement is to pursue the HF calculations with more vigor. Although reference 3 gives an excellent treatment of the HF problem the authors of that paper suggest the following improvements which could bring the binding energy in line with the experimental value: First, the problem should be done in a doubly self-consistent way, and second, more nodes should be

³²R. P. Lynch and T. T. S. Kuo, Nucl. Phys. A95 (1967) 561

included in the expansion of the HF wave functions. Efforts along these lines have been initiated.

The second explanation of the difference in the experimental and calculated results is directly related to the nucleon-nucleon potentials which are currently in use. Since the spectrum calculations of Kuo and Brown⁷ rely basically on the long range part of the potential and give excellent agreement with experiment, it is believed that the poor binding energy results may be due to the short range part of the potential. In particular a potential with a smaller hard core radius or a soft core would improve the binding energy results.

Along these same lines it has been suggested by several authors^{33, 34} that one should by pass the use of potentials and attempt to calculate the t-matrix for finite nuclei by working directly with the experimental phase shifts. This avenue of approach would be very desirable although new calculational techniques would have to be devised, and the attempts to date--though admittedly initial attempts--have not shed any light on how to handle the Pauli operator in conjunction with the phase shifts.

³³J. P. Elliot, H. A. Avromatis, E. A. Sanderson, Phys. Letters 24B (1967) 358

³⁴Koltun, unpublished

Finally, there is the difficult question of the convergence of the Bethe-Goldstone expansion and the effect of higher order terms in finite nuclei. Bethe and Rajaraman³⁵ have shown that three body correlations are important in nuclear matter and these contributions will also have to be examined for finite nuclei.

In summary it is believed that the Hartree-Fock, higher order cluster effects, and better potentials individually would contribute at best 1 MeV per nucleon. So collectively one may expect an improvement of the order of 2 to 3 MeV which would still leave the binding energy too small by roughly 2 MeV. These crude estimates indicate that it may finally be necessary to include specifically three body forces in order to get good agreement with the experimental binding energies.

³⁵R. Rajaraman and H. Bethe, Rev. Mod. Phys. 39 (1967)

APPENDIX A

TREATMENT OF HARD-CORE

In this Appendix an approximate expression for the hard core contribution to the t-matrix will be discussed. Once the BG wave-function, ψ , has been obtained the t-matrix is calculated from

$$\langle \phi_n | t | \phi_m \rangle = \int_0^{\infty} \phi_m' v \psi_m d\rho = I_1 + I_2 \quad (1)$$

where

$$I_1 = \lim_{\epsilon \rightarrow 0} \int_0^{\rho_c + \epsilon} \phi_m' v_{\text{core}} \psi_m d\rho \quad (2)$$

$$I_2 = \lim_{\epsilon \rightarrow 0} \int_{\rho_c + \epsilon}^{\infty} \phi_m' v \psi_m d\rho \quad (3)$$

The integral, I_2 , is straightforward to evaluate using standard numerical integration. The first integral, I_1 , presents some difficulties since v is infinite for $\rho \leq \rho_c$; however, by using the BG

equation it is possible to approximate $v_{\text{core}} \psi_n$. From the BG equation for $r \leq r_c$ we have

$$v_{\text{core}} \psi_n = (E_n - H_0) \psi_n - (E_n - E_n^0) \phi_n \langle \phi_n | \psi_n \rangle + \sum_a C_a^* \phi_a \langle \phi_a | \psi_n \rangle \quad (4)$$

Using equation (4) in (2) gives

$$I_1 = \lim_{\epsilon \rightarrow 0} \left\{ \int_0^{r_c + \epsilon} [\phi_n (E_n - H_0) - (E_n - E_n^0) \langle \phi_n | \psi_n \rangle \phi_n] \phi_n dr \right. \\ \left. + \sum_a C_a^* \langle \phi_a | \psi_n \rangle \int_0^{r_c + \epsilon} \phi_n(r) \phi_a(r) dr \right\} \quad (5)$$

It has been found in actual calculations that the last two terms in equation (5) are small compared to the first term. This is directly related to the fact that

$$\int_0^{r_c + \epsilon} \phi_n \phi_n dr \approx 10^{-3} \quad (6)$$

Therefore,

$$I_1 \cong \lim_{\epsilon \rightarrow 0} \int_0^{r_c + \epsilon} \phi_n (E_n - H_0) \psi_n dr \quad (7)$$

Since ψ_n is zero for $f \leq f_c$ this integral is zero except at $f = f_c$ where $\frac{d^2\psi}{df^2}$ has a δ -function singularity. Then,

$$I_1 \approx \lim_{\epsilon \rightarrow 0} \frac{\pi^2}{2m} \int_{f_c - \epsilon}^{f_c + \epsilon} \phi_{n'} \frac{d^2\psi_n}{df^2} df \quad (8)$$

Integrating by parts gives

$$I_1 \approx \lim_{\epsilon \rightarrow 0} \frac{\pi^2}{2m} \left\{ \phi_{n'} \frac{d\psi_n}{df} \Big|_{f_c - \epsilon}^{f_c + \epsilon} - \int_{f_c - \epsilon}^{f_c + \epsilon} \frac{d\phi_{n'}}{df} \frac{d\psi_n}{df} df \right\}$$

Since $\frac{d\phi}{df}$ and $\frac{d\psi}{df}$ are both finite quantities, the second term goes to zero as $\epsilon \rightarrow 0$. Therefore, we have

$$I_1 \approx \frac{\pi^2}{2m} \phi_{n'} \frac{d\psi_n}{df} \Big|_{f=f_c} \quad (9)$$

Equation (9) can be evaluated numerically and I_1 has been added to all calculations of the t-matrix.

APPENDIX B*

NUMERICAL METHODS

In this appendix the numerical methods used to solve the BG equation are discussed in detail. The method used is basically an extension of the Fox-Goodwin³⁶ method. In the past, the Fox-Goodwin method has been applied to differential equations, and to the author's knowledge, it has never been used to solve integro-differential equations.

After dropping all subscripts in the BG equation, the integro-differential equation which was solved is of the form

$$\begin{aligned} \left[\lambda - \frac{1}{2} \lambda^2 - V(\beta) \right] u(\beta) &= (\lambda - \lambda') R(\beta) \langle R/u \rangle \\ &- \sum_{\alpha} c^{\alpha} R^{\alpha}(\beta) \langle R^{\alpha}/u \rangle \end{aligned} \quad (1)$$

By expanding u and u' in a Taylor series and performing a little algebra, we get the following three-point equation

*The author is indebted to Dr. P. Signell for initially suggesting the method for solving differential equations which was ultimately extended to treat integro-differential equations.

³⁶L. Fox and A. Goodwin, Proc. of Cambridge Phil. Soc. 45 (1949) 373.

$$(u_{j+1} - \frac{\Delta^2}{12} u_{j+1}'') - (2u_j + \frac{5}{6}\Delta^2 u_j'') + (u_{j-1} - \frac{\Delta^2}{12} u_{j-1}'') = 0 \quad (2)$$

where Δ is the mesh width and j denotes the j^{th} mesh point. From equation (1) expressions for u_j'' , u_{j+1}'' , and u_{j-1}'' can be obtained, and when these are substituted into equation (2), we get

$$u_{j+1} A_j + u_j B_j + u_{j-1} C_j = (\lambda - \lambda^0) \frac{\Delta^2}{12} [R_{j+1} + 10R_j + R_{j-1}] \langle R|u \rangle \\ - \frac{\Delta^2}{12} \left[\sum_a C_a^{\sim} (R_{j+1}^{\sim} + 10R_j^{\sim} + R_{j-1}^{\sim}) \langle R^{\sim}|\psi|u \rangle \right] \quad (3)$$

where

$$A_j = 1 + \frac{\Delta^2}{12} (\lambda - V_{j+1}) \\ B_j = -2 + \frac{5}{6} \Delta^2 (\lambda - V_j) \\ C_j = 1 + \frac{\Delta^2}{12} (\lambda - V_{j-1}) \quad (4)$$

Let u^* be a trial wave function and δu be the change in the trial wave function. Then

$$u_j = u_j^* + \delta u_j \quad (5)$$

After substituting equation (5) into equation (3) we get

$$\begin{aligned} & A_j u_{j+1}^* + B_j u_j^* + C_j u_{j-1}^* + A_j \delta u_{j+1} + B_j \delta u_j + C_j \delta u_{j-1} \\ &= (\lambda - \lambda^0) \frac{\Delta^2}{12} [R_{j+1} + 10 R_j + R_{j-1}] [\langle R|u \rangle + \langle R|\delta u \rangle] \quad (6) \\ & - \frac{\Delta^2}{12} \left[\sum_a C^a (R_{j+1}^a + 10 R_j^a + R_{j-1}^a) \right] [\langle R^a|u \rangle + \langle R^a|\delta u \rangle] \end{aligned}$$

At this point the plausible assumption is made that

$$\langle R|\delta u \rangle \ll \langle R|u^* \rangle$$

and

$$\langle R^a|\delta u \rangle \ll \langle R^a|u^* \rangle$$

Even though a given u_j may be comparable to a given δu_j , these assumptions imply that on the average δu is much less than u^* .

The validity of these assumptions is ultimately justified by the rapid convergence of the solutions. When convergence is obtained, $\delta u = 0$, and there is no question of approximation. The final results can be made as accurate as desired, limited only by the accuracy of the computer.

After dropping the small terms in equation (6) we get

$$Q_j + A_j \delta u_{j+1} + B_j \delta u_j + C_j \delta u_{j-1} = 0 \quad (7)$$

where

$$\begin{aligned} Q_j &\equiv A_j u_{j+1}^* + B_j u_j^* + C_j u_{j-1}^* - (\lambda - \lambda^0) \frac{\Delta^2}{12} [R_{j+1}^* + 10R_j^* + R_{j-1}^*] \langle R | u^* \rangle \\ &+ \frac{\Delta^2}{12} \left[\sum_a C_a^* (R_{j+1}^* + 10R_j^* + R_{j-1}^*) \langle R^* | u^* \rangle \right] \end{aligned} \quad (8)$$

Next let

$$\delta u_j = F_j + H_j \delta u_{j+1} \quad (9)$$

Then equation (7) becomes

$$Q_j + A_j \delta u_{j+1} + B_j \delta u_j + C_j (F_{j-1} + H_{j-1} \delta u_j) = 0 \quad (10)$$

By comparing equations (9) and (10) term by term, we get

$$F_j = - (C_j F_{j-1} + Q_j) (B_j + C_j H_{j-1})^{-1} \quad (11)$$

$$H_j = - A_j (B_j + C_j H_{j-1})^{-1} \quad (12)$$

The A_j , B_j , C_j and Q_j are well defined numerical quantities, and the F_j and H_j can be determined provided F_0 and H_0 are known. F_0 and H_0 can be determined from the boundary conditions at the hard core, viz. $u(\text{Core}) = u^*(\text{Core}) = 0$. Then

$$\delta u_0 = 0 = F_0 + H_0 \delta u_1 \quad (13)$$

Since F_0 and H_0 are independent quantities F_0 and H_0 must be zero in order to satisfy equation (13).

Since the ultimate aim is to calculate each of the δu_j 's from equation (9), we now need to know δu_N where N denotes the

last mesh point. δu_N is found from the asymptotic form of the BG equation. From equation (1), we have

$$u_N \propto e^{-[\Delta(N-1)]^2/2} = e^{-s^2/2} \quad (14)$$

and

$$u_{N+1} \propto e^{-[\Delta N]^2/2} \quad (15)$$

From equations (14) and (15) we get

$$\delta u_N = \delta u_{N+1} e^{-\Delta^2(1-2N)/2} \quad (16)$$

Combining equation (16) and (9) gives

$$\delta u_{N+1} = -F_N \left(H_N - e^{-\Delta^2(1-2N)/2} \right)^{-1} \quad (17)$$

Since the F_j 's and H_j 's and δu_{j+1} 's are known, all of the δu_j 's can now be obtained from equation (9). Once the δu_j 's are known a new trial wave function u^{**} can be computed using equation (5).

After u^{**} is obtained the whole procedure is repeated with u^{**}

replacing u^* . The iterative process is terminated when $\sum \delta u_j$ is less

than some arbitrarily small number. Usually the convergence is quite rapid if one is sufficiently careful in choosing an initial trial wave function. Even with "bad" trial wave functions the convergence is satisfactory.

In practice the initial trial wave function is chosen to be of the form

$$u(\rho) = (1 - \rho/\rho_c) R(\rho) \quad (18)$$

This form of the wave function fulfills the necessary requirements at the hard core and asymptotically.

The method outlined above is applicable to both coupled and uncoupled equations. For the case of coupled equations the only difference is that the wave function, u , is a vector quantity and the expression for the A 's, B 's, C 's, H 's, F 's etc. are matrices.

For completeness the method used to solve the ordinary differential equation will be outlined. The form of this equation is

$$\left[\lambda + \frac{d^2}{d\rho^2} - V(\rho) \right] u(\rho) = 0 \quad (19)$$

where λ is now an eigenvalue to be obtained along with the wave function, u . Equation (19) is used to find u''_j , u''_{j+1} and u''_{j-1} and

these expressions are substituted into equation (2) to give

$$u_{j+1} A_j + u_j B_j + u_{j-1} C_j = 0 \quad (20)$$

where A_j , B_j , and C_j are defined by equation (4). Now let u^* be a trial wave function and λ^* be a trial eigenvalue. Then

$$u_j = u_j^* + \delta u_j \quad (21)$$

$$\lambda = \lambda^* + \delta \lambda \quad (22)$$

after substituting equations (21) and (22) into equation (20) we get

$$Q_j + D_j \delta \lambda + A_j^* \delta u_{j+1} + B_j^* \delta u_j + C_j^* \delta u_{j-1} = 0 \quad (23)$$

where terms of the order $\delta u \delta \lambda$ have been dropped and

$$Q_j \equiv u_{j+1}^* A_j^* + u_j^* B_j^* + u_{j-1}^* C_j^* \quad (24)$$

$$D_j \equiv \frac{a^2}{12} [u_{j+1}^* + 10 u_j^* + u_{j-1}^*] \quad (25)$$

Next let

$$\delta u_j = F_j + H_j \delta u_{j+1} + E_j \delta \lambda \quad (26)$$

Then substitute equation (26) into equation (23) and rearrange terms to get

$$\delta u_j = -\frac{1}{d_j} [Q_j + C_j^* F_{j-1} + H_j^* \delta u_{j+1} + (D_j + C_j^* E_{j-1}) \delta \lambda] \quad (27)$$

where

$$d_j \equiv B_j^* + C_j^* H_{j-1} \quad (28)$$

By comparing equation (27) and (26) term by term we get

$$F_j = -(Q_j + C_j^* F_{j-1})/d_j$$

$$H_j = -H_j^*/d_j$$

$$E_j = -(C_j^* E_{j-1} + D_j)/d_j$$

(29)

The A_j , B_j , C_j , D_j and Q_j are well defined numerical quantities and the F_j , H_j , and E_j can be determined if F_0 , H_0 and E_0 are known. F_0 , H_0 , and E_0 can be determined from the boundary condition at the coare, viz., $u(\text{core})=u^*(\text{core})=0$. Then

$$\delta u_0 = F_0 + H_0 \delta u_1 + E_0 \delta \lambda = 0 \quad (30)$$

and since F_0 , H_0 and E_0 are independent quantities F_0 , H_0 , and E_0 must be zero in order to satisfy equation (30).

Since the ultimate aim is to calculate each of the δu_j 's and $\delta \lambda$ we need to know δu_N where N denotes the last mesh point. As was done earlier δu_N is found from the asymptotic boundary condition. For this case we simply require that the wave function be zero at large distances. This makes δu_N and δu_{N+1} zero. Therefore, from equation (26) we get

$$\delta \lambda = -F_j/E_j \quad (31)$$

The solution is now complete since all the F_j 's, H_j 's, and E_j 's are well defined in terms of the trial wave function and trial eigenvalue, and $\delta \lambda$ and the δu_j 's can be calculated using equation (31)

and (26). Once the $\delta\lambda$ and δu_j 's are determined a new eigenvalue λ^{**} and a new wave function u^{**} can be computed and the whole procedure is repeated until $\sum \delta u_j$ and $\delta\lambda/\lambda$ are arbitrarily small.

APPENDIX C

PARAMETERS AND PROPERTIES OF THE NUCLEON-NUCLEON POTENTIAL

The form of the HJ and BGT potential

$$V(r) = V_c(r) + V_s(r) \bar{J} \cdot \bar{S} + V_{LL}(r) L_{12} + V_T(r) S_{12}$$

where

$$\bar{J} \cdot \bar{S} = \frac{1}{2} [j(j+1) - l(l+1) - s(s+1)]$$

$$L_{12} = \left[\delta_{lj} + \vec{\sigma}_1 \cdot \vec{\sigma}_2 \right] l(l+1) - (\bar{J} \cdot \bar{S})^2 \quad (\text{For HJ})$$

$$L_{12} = 0 \quad (\text{For BGT})$$

$$S_{12} = \frac{3}{r^2} (\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2$$

The radial dependence of the HJ potential is given by

$$V(r) = +\infty \quad r \leq r_c$$

$$V_c(r) = .08 \left(\frac{1}{3} \mu \right) (\vec{E}_1 \cdot \vec{E}_2) Y(r) [1 + a_c Y(r) + b_c Y^2(r)]$$

$$V_{LS}(r) = \mu G_{LS} Y^2(r) [1 + b_{LS} Y(r)]$$

$$V_{LL}(r) = \mu G_{LL} r^{-2} Z(r) [1 + a_{LL} Y(r) + b_{LL} Y^2(r)]$$

where

$$Y(r) = \frac{e^{-r}}{r}$$

$$Z(r) = \left(1 + \frac{3}{r} + \frac{3}{r^2} \right) Y(r)$$

μ is the pion mass (139.4 MeV), and x is measured in $\hbar/\mu c = 1.415$ fm.

The hard core radius in all states is $0.343 \hbar/\mu c$, and corresponds

to $r_c = .485$ fm. The parameters for the HJ potential are given in

Table VI.

TABLE VI. --Parameters for Hamada-Johnston potential.

State	a_c	b_c	a_T	b_T	G_{LS}	b_{LS}	G_{LL}	a_{LL}	b_{LL}
Singlet even	+8.7	+10.6	0	0	0	0	-0.000891	+0.2	-0.2
Triplet odd	-9.07	+3.48	-1.29	+0.55	+0.1961	-7.12	-0.000891	-7.26	+6.92
Triplet even	+6.0	-1.0	-0.5	+0.2	+0.0743	-0.1	+0.00267	+1.8	-0.4
Singlet odd	-8.0	+12.0	0	0	0	0	-0.00267	+2.0	+6.0

The radial dependence for all states of the BGT potential is given by

$$V(r) = +\infty \quad r \leq r_c$$

$$= -\frac{\sqrt{6}}{4r} e^{-4r} \quad r > r_c$$

The parameters for the BGT potential are given in Table VII.

TABLE VII. --Parameters of the Brueckner-Gammel-Thaler potential.

Parity	3V_c	3M_c	1V_c	1M_c	3V_t	3M_t	${}^3V_{ls}$	${}^3M_{ls}$
+	877.4	2.091	434.0	1.45	159.4	1.045	5000	3.7
-	14.0	1.0	-130.0	1.00	-22.0	0.80	7315	3.7

APPENDIX D

DERIVATION OF BINDING ENERGY

In this appendix the expression for the total energy of a closed-shell nucleus is derived in terms of the reduced matrix elements.

The potential energy to first order is given by

$$P = \frac{1}{2} \sum_{\substack{\text{occupied} \\ n_1 l_1 j_1 J M_1 \\ n_2 l_2 j_2 T M_2}} (1 + \delta_{n_1 l_1 j_1, n_2 l_2 j_2}) \quad (1)$$

$$\times \langle (l_1 l_1) j_1 (l_2 l_2) j_2 J M_1 T M_2 m_1 m_2 | t | (l_1 l_1) j_1 (l_2 l_2) j_2 J M_1 T M_2 m_1 m_2 \rangle$$

Where both the ket and bra are the proper normalized, anti-symmetric wave functions given by equation (4) Chapter II. After substituting the transformed two particle state vectors into equation (1) and using the orthogonality of the center-of-mass wave functions the following is obtained:

$$\begin{aligned}
P = & \frac{1}{4} \sum_{\substack{\text{OCCUPIED} \\ m_1 l_1 j_1 J M_J \\ m_2 l_2 J_2 M_J}} \sum_{\substack{S \Lambda \\ m_1 N L}} T_{S \Lambda J}^{l_1 l_2 j_1 j_2} \langle m_1 l_1 m_2 l_2 | m_1 N L, \Lambda \rangle \\
& \times \sum_j [1 - (-1)^{l+s+T}] \Lambda_{J L \Lambda}^{l s j} \sum_{m_j m_L} C(j L m_j m_L | J M_J) \\
& \times \sum_{\substack{s' \Lambda' m' l' \\ s' \Lambda' J}} T_{s' \Lambda' J}^{l_1 l_2 j_1 j_2} \langle m' l' N L, \Lambda' | m_1 l_1 m_2 l_2 \rangle [1 - (-1)^{l'+s'+T}] \\
& \times \sum_{j' m_{j'}} \Lambda_{J L \Lambda'}^{l' s' j'} C(j' L m_{j'} m_L | J M_J) \langle (l s) j' m_{j'} m_L | t(N L) | (l' s') j' m_{j'} m' \rangle
\end{aligned} \tag{2}$$

Next we split the wave function into its radial and angular parts, use the fact that the interaction is diagonal in S , j , m_j , and utilize the orthogonality of the Clebsch-Gordan coefficients to obtain

$$\begin{aligned}
P &= \frac{1}{j} \sum_{m, l, m_l} \sum_{T S \Lambda \Lambda'} \sum_{m' l' m'_l} (2T+1) \langle m l N L, \Lambda | m, l, m_l, l_z \rangle \\
&\quad \times \langle m, l, m_l, l_z | m' l' N L, \Lambda \rangle [1 - (-1)^{l+l'+T}] [1 - (-1)^{l'+S+T}] \\
&\quad \times \langle m l s j | T(NL) | m' l' s j \rangle \sum_J (2J+1) \Lambda_{J L \Lambda'}^{l s j} \quad (3) \\
&\quad \times \sum_{j_1 j_2} T_{S \Lambda J}^{l_1 l_2 j_1 j_2} T_{S \Lambda' J}^{l'_1 l'_2 j'_1 j'_2}
\end{aligned}$$

For a closed-shell nucleus the sum over $j_1 j_2$ can be eliminated by using the properties of the LS-jj transformation coefficients. If we also use the properties of the 6-j symbols, viz.,

$$\sum_J (2J+1) \Lambda_{J L \Lambda}^{l s j} \Lambda_{J L \Lambda'}^{l' s' j'} = (2j+1)(2\Lambda+1) \delta_{j j'} / (2J+1) \quad (4)$$

then we get

$$\begin{aligned}
P = & \frac{1}{2} \sum_{T S j} \sum_{m' N L m'} (2T+1) [1 - (-1)^{l+s+T}] (2j+1) \\
& \times \langle m l s j | t(NL) | m' l s j \rangle \sum_{m_1 l_1 m_2 l_2 1}^{\text{OCCUPIED}} \frac{(2l+1)}{(2l+1)} \\
& \times \langle m l N L, 1 | m_1 l_1 m_2 l_2 \rangle \langle m_1 l_1 m_2 l_2 | m' l N L, 1 \rangle
\end{aligned} \tag{5}$$

Finally using the implicit energy relations of the Brody-Moshinsky brackets, viz., $2n_1 + l_1 + 2n_2 + l_2 = 2n + l + 2n + L$ we get

$$\begin{aligned}
P = & \frac{1}{2} \sum_{T S j} \sum_{m' N L} (2T+1) (2j+1) \langle m l s j | t(NL) | m' l s j \rangle \\
& \times [1 - (-1)^{l+s+T}] \sum_{m_1 l_1 m_2 l_2 1}^{\text{OCCUPIED}} \frac{(2l+1)}{(2l+1)} |\langle m_1 l_1 m_2 l_2 | m l N L, 1 \rangle|^2
\end{aligned} \tag{6}$$

We now need to know the kinetic energy of the particles. This is given by $\sum_{m_i} \langle m_i | T | m_i \rangle$ where T is the single particle kinetic energy operator and $|n_0\rangle$ denotes the unperturbed harmonic oscillator state vector. It is easily shown that the diagonal matrix elements of the kinetic energy is one half the total energy of the harmonic oscillator. For ^{16}O we only need to sum over the os and

op shells, and since there are 4 particles in the os shell all with kinetic energy $\frac{3}{4}\hbar\omega$ and 12 particles in the op shell all with kinetic energy $\frac{5}{4}\hbar\omega$, the total kinetic energy is $18\hbar\omega$. This is then added to equation (7) to give the total ground state energy of ^{16}O .

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