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A NEW METHOD FOR CALCULATION OF EIGENSTATES FOR A SYSTEM OF A CORE AND TWO VALENCE NUCLEONS

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Новый метод вычисления собственных состояний системы, состоящей из кора и двух валентных нуклонов

Предложен метод для вычисления собственных функций и собственных значений системы, состоящей из кора и двух валентных нуклонов. Метод состоит в замене точного потенциала в уравнении Липпмана-Швингера приближенным потенциалом, представляющим собой сумму сепарабельных членов. Для приближенного потенциала уравнение Липпмана-Швингера решается точно. В качестве базиса для разложения выбираются функции гармонического осциллятора. Волновая функция, полученная в данном методе, имеет правильную "трехчастичную" асимптотику и приближенную"двухчастичную".Численные расчеты проводились для ядра ^{18}O. Среднее поле выбиралось вудс-саксоновского типа, остаточные взаимодействия - в виде потенциала Юкавы. Проведенное сравнение с результатами, полученными обычной процедурой диагонализации, показало, что волновая функция данного метода имеет значительно лучшее асимптотическое поведение.

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A New Method for Calculation of Eigenstates for a System of a Core and Two Valence Nucleons

A method for calculation of eigenvalues and eigenstates for a system of a core and two valence nucleons is suggested. It consists in approximating the potential by a sum of separable terms, for which the Lippman-Schwinger equation is solved exactly. The wave functions have the exact "three-particle" asymptotic form and approximate "two-particle" asymptotics.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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It is well-known, that the nuclear transfer reactions take place in the surface region of nuclei. A more exact determination of the region must depend on the reaction in question, in subbarrier proton stripping, e.g., the region between one and four or five nuclear radii gives the main contribution. The density of nucleons is small for such distances, and it is therefore not surprising, that in spectroscopic calculations the contributions of these regions can be neglected, but in calculations of transfer amplitudes, they are essential.

The asymptotic behaviour of the form factors for one particle transfer can in general be derived from simple considerations [1]. But an expression for the asymptotics of two-nucleon transfer form factors has not yet been derived; in the natural three-body wave function approximation Mercuriev [2] recently has obtained its asymptotic form and it turns out to be a rather complicated function of the coordinates.

A number of methods have been suggested for the calculations of these two nucleon transfer form factors, but it is obvious that only two of them [3,4], which use expansions on a complete set of functions, can, by carrying the expansion sufficiently far, approximate the asymptotic part of the form factor sufficiently well. In one of these methods, the basis states are of harmonic oscillator type [3] in the other they are the Sturm-Liouville functions [4]. It should be noted, that although the method of ref. [3] in principle must lead to the correct result, in realistic calculations it implies the diagonalization of matrices of extremely high rank (larger than 1000), i.e., the convergence of the expansion is slow. With the Sturm-Liouville expansion method, the series converge

faster, but each of the basis functions and the corresponding coefficients of coordinate transformation must be calculated numerically. In this respect the expansion on harmonic oscillator functions has some advantages, since the functions themselves and many integrals and transformation coefficients can be expressed analytically. The aim of the present work is to improve the rapidity of the convergence working with the harmonic oscillator basis. A method for this was suggested in the work [5].

Let us look at the simplest case of two identical particles interacting with each other and with an inert core. The fundamental assumption is, that the interaction between the particles is so weak, that a bound state of two particles without the core does not exist. The inert core is considered to be infinitely heavy, so the Hamiltonian is that of two interacting particles in a potential well. The nearest physical analogue is the system of two identical particles outside a doubly closed shell.

So, in this model, the wave functions ψ_A of the nucleus A are represented as products

$$\psi_A(\bar{r}_1, \bar{r}_2, \xi) = \psi_{A-2}(\xi)\psi(\bar{r}_1, \bar{r}_2) .$$

This means, that we do not include polarizations of the (A-2) core by the valence nucleons. Therefore, the problem is reduced to a 3-body problem, but we must here take the Pauli principle into account, and in this way our model differs from the usual 3-body problems.

So, we want to solve the Schrödinger equation

$$[H_0 + \lambda(V(r_1) + V(r_2)) + \gamma V_{12}(\bar{r}_{12}) - E]\psi = 0 , \qquad (1)$$

where V_{12} is the residual interaction and $V(r_1)+V(r_2)$ is the nuclear potential.

In principle, any of the quantities λ, γ and E can be considered the eigenvalue of equation (1). If, e.g., the depth of the potential well, λ, and the energy E are known, γ will be the eigenvalue.

Let V be the sum of the potential and the residual interaction

$$V = \lambda(V(r_1) + V(r_2)) + \gamma V_{12}(\bar{r}_{12}) . \qquad (2)$$

We shall now approximate V by a sum of separable terms

$$V \approx V^N_{sep} = \sum_{\mu\nu}^{N} |\mu><\mu|V|\nu><\nu| , \qquad (3)$$

where $|\mu> \equiv |\mu_1>|\mu_2>$, and the ket vectors $|\mu_{1,2}>$ are defined by their form factors, e.g., in the momentum space

$$<k|n\ell jm> = R_{n\ell_j}(k)[Y_\ell(\hat{k}) \cdot \chi(s)]^j_m , \qquad (4)$$

N is the number of terms in the basis. The exactness of the approximation (3) obviously depends on N; for $N \to \infty$ the approximate potential V^N_{sep} becomes identical to V. For bound states equation (1) can now using V^N_{sep} be approximated by

$$\begin{aligned} |\psi> &= G_0(E) \sum_{\mu\nu} |\mu> V_{\mu\nu} <\nu|\psi> = \\ &= G_0(E) \sum_{\mu\nu} |\mu> V_{\mu\nu} C_\nu , \end{aligned} \qquad (5)$$

where $G_0(E) = \dfrac{1}{E - H_0}$

is the Green operator.

Multiplying equation (5) with $<\sigma|$ we obtain a system of equations for the coefficients $C_\nu = <\nu|\psi>$

$$\sum_\nu \{\delta_{\sigma\nu} - \sum_\mu <\sigma|G_0(E)|\mu> V_{\mu\nu}\} C_\nu = 0 . \qquad (6)$$

So, the condition for solution of (6)

$$|\delta_{\sigma\nu} - \sum_\mu <\sigma|G_0(E)|\mu> V_{\mu\nu}| = 0 \qquad (7)$$

gives us the eigenvalues, e.g., E_i, and by use of (6) the corresponding coefficients $C^{(i)}_\nu$. In this case the

$C_\nu^{(i)}$ are not eigenvector components of a symmetric matrix, but nevertheless, the eigenfunctions $|\psi_i>$, which belong to different eigenvalues E_i, are mutually orthogonal. Actually, we have

$$|\psi_1> = \frac{1}{E_1 - H_0} \sum_{\mu\nu} |\mu> V_{\mu\nu} C_\nu^{(1)},$$
$$|\psi_2> = \frac{1}{E_2 - H_0} \sum_{\mu\nu} |\mu> V_{\mu\nu} C_\nu^{(2)}. \quad (8)$$

Then the overlap $<\psi_1|\psi_2>$ is

$$<\psi_1|\psi_2> = \sum_{\substack{\mu\nu \\ ij}} <\mu| \frac{1}{E_1 - H_0} \cdot \frac{1}{E_2 - H_0} |i> V_{\mu\nu} C_\nu^{(1)} V_{ij} C_j^{(2)}. \quad (9)$$

Using the identity

$$\frac{1}{E_1 - H_0} \cdot \frac{1}{E_2 - H_0} = \frac{1}{E_2 - E_1} \left(\frac{1}{E_1 - H_0} - \frac{1}{E_2 - H_0} \right) (E_2 \neq E_1)$$

and the equation (6) for the coefficients $C_\nu^{(1)}$ and $C_j^{(2)}$, we obtain

$$<\psi_1|\psi_2> = \frac{1}{E_2 - E_1} \sum_{ij} (C_i^{(1)} V_{ij} C_j^{(2)} - C_i^{(2)} V_{ij} C_j^{(1)}) = 0$$

for $E_2 \neq E_1$. For $E_2 = E_1$ we get, of course, $<\psi_1|\psi_2> = 1$.

It is easy to show, that the wave functions (5) can be chosen antisymmetric in the coordinates of the two valence nucleons, but still, they should also obey the Pauli principle with respect to all other nucleons of the system.

In the ordinary shell model, this is easily achieved. It is simply assumed, that the nucleons of the closed and non-closed shell are moving in the same average field. Then the two-nucleon wave function is expanded over the wave functions of independent particles, moving in the average field, excluding such states which are occupied in the core. This means that in this approximation, the residual interactions are neglected for the core particles.

For double magic nuclei, this approximation may be sufficiently good, and we shall here make the same assumption using the method, suggested in [4].

Let us introduce the effective Hamiltonian

$$\tilde{H} = H + T \sum_i |i><i|, \quad (10)$$

where the $|i>$ are all such two-nucleon states, where at least one of the nucleons is in an occupied orbit * .

Now, the solution of the Schrödinger equation with the effective Hamiltonian (10) can be written

$$|\tilde{\psi}> = |\psi> + G(E) T \sum_i |i><i|\tilde{\psi}>,$$
$$G(E) = (E - H)^{-1} \quad (11)$$

from which we obtain

$$<i|\tilde{\psi}> = \sum_j <i| (1 - TG(E))^{-1} |j><j|\psi>. \quad (12)$$

Therefore, for $T \to \infty$, $<i|\tilde{\psi}> \to 0$. In practice, when T is sufficiently large ($T \geq 10^4 \cdot 2m/\hbar$ fm^{-2}), the wave function $|\tilde{\psi}>$ will be orthogonal to the occupied states of the core, within the requirements of accuracy met elsewhere in the calculations.

We shall now discuss the asymptotic behaviour of the wave functions calculated by this method. It is easy to show (see Appendix) that the "three-particle" asymptotics (in Merkuriev's terminology) looks as

$$<r_1 r_2|\psi> \approx \frac{\exp\{-\sqrt{\frac{2m}{\hbar^2}|E|}\,\rho\}}{\rho^{5/2}} u(\hat{\rho}), \quad (13)$$

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* The occupied states should be those of the nuclear Woods-Saxon field, in the present calculation, we identified the only occupied state with harmonic oscillator 1s state.

$$\rho = \sqrt{r_1^2 + r_2^2}, \quad \hat{\rho} = \frac{\bar{\rho}}{\rho}$$

and coincidences with the results from ref.[2]. Strictly speaking in Merkuriev's sense our wave function has no two-particle asymptotics. Let us consider, however the overlap integral $\langle R_{n\ell_j}(\bar{r}_1)|\psi(\bar{r}_1,\bar{r}_2)\rangle$, where $R_{n\ell_j}(\bar{r}_1)$ is one-particle wave function in the potential $V(r_1)$. Obviously, for an exact ψ its asymptotic form should be

$$\langle R_{n\ell_j}(\bar{r}_1)|\psi(\bar{r}_1,\bar{r}_2)\rangle \sim \frac{\exp\{-\sqrt{\frac{2m}{\hbar^2}}|E-E_{n\ell_j}|r_2\}}{r_2}, \quad r_2 \to \infty . \tag{14a}$$

For our ψ it has a rather complicated form, for the lowest term $\psi_{1s\,1s}$ it is calculated in the Appendix and it gives

$$\langle R_{1s}(\bar{r}_1)|\psi_{1s1s}(\bar{r}_1,\bar{r}_2)\rangle \sim \frac{\exp\{-\sqrt{\frac{2m}{\hbar^2}}|E|\,r_2\}}{r_2^{3/2}} . \tag{14b}$$

For the complete wave function, however, the asymptotic region can be divided into two intervals

a) $R_0 < r < \beta R_0$,
b) $\beta R_0 < r$,

where R_0 is the radius of the mean field, whereas β depends on the number of configurations $(n\ell j)$ taken into account in the calculation and in a) the function is described by (14a) while for b) (14b) holds. It is natural to expect, and it is confirmed by the calculations, that the interval a) becomes larger, when the number of configurations is enlarged. Accordingly the wave functions of the method suggested here have the correct three particle asymptotic form and a form which approximates the two-particle asymptotic; this is just the advantage of this method as compared to the usual method of expansion in oscillator functions.

Below, we shall give a short description of the techniques used in calculation of some of the integrals which are met in these calculations.

The radial oscillator function is

$$R_{n\ell}(r) = N_{n\ell}\, r^{\ell} \exp\{-\frac{1}{2}\lambda r^2\} L_n^{\ell+1/2}(\lambda r^2) , \tag{15}$$

$$N_{n\ell} = \left(\sqrt{\frac{2}{\pi}} \cdot \frac{2^n}{n!} \cdot \frac{(2\lambda)^{\ell+3/2}}{(2n+2\ell+1)!!!}\right)^{1/2}, \lambda = \frac{m\omega}{\hbar} = \frac{1}{b^2}, \tag{16}$$

where $L_n^{\ell+1/2}$ is a Laguerre polynomial. In the momentum representation the wave function $R_{n\ell}(k)$ has the same form as (15) except fot a phase $(-1)^n \cdot i^{\ell}$ and a factor $\lambda_k = \frac{1}{\lambda}$ in the place of λ.

The matrix elements of the two-particle Green function are conveniently calculated in the momentum representation, since it is diagonal in this representation. Let us write the two-particle wave functions as

$$|n_1\ell_1 j_1, n_2\ell_2 j_2; jm\rangle = \sum_{m_1 m_2} \langle j_1 m_1 j_2 m_2|jm\rangle \times$$
$$\times R_{n_1\ell_1}(k_1) R_{n_2\ell_2}(k_2)\, Y_{\ell_1 j_1}^{m_1}(\hat{k}_1) Y_{\ell_2 j_2}^{m_2}(\hat{k}_2) , \tag{17}$$

then

$$M = \langle n_1\ell_1 j_1, n_2\ell_2 j_2; jm|G_0(E)|n_1'\ell_1' j_1', n_2'\ell_2' j_2'; j'm'\rangle$$

$$= \delta_{\ell_1\ell_1'}\delta_{\ell_2\ell_2'}\delta_{j_1 j_1'}\delta_{j_2 j_2'}\delta_{jj'}\delta_{mm'} R(n_1 n_2 n_1' n_2' \ell_1 \ell_2),$$

$$R(n_1 n_2 n_1' n_2' \ell_1 \ell_2) = \langle R_{n_1\ell_1}(k_1) R_{n_2\ell_2}(k_2)|$$

$$\frac{1}{E - \frac{\hbar^2 k_1^2}{2m} - \frac{\hbar^2 k_2^2}{2m}} |R_{n_1'\ell_1'}(k_1) R_{n_2'\ell_2'}(k_2)\rangle . \tag{18}$$

These integrals are calculated by using the following relations

$$\frac{1}{a} = \int_0^\infty \exp\{-ax\}dx,$$

$$\frac{1}{|E| + \frac{\hbar^2}{2m}(k_1^2+k_2^2)} = \int_0^\infty \exp\{-\alpha(|E| + \frac{\hbar^2 k_1^2}{2m} + \frac{\hbar^2 k_2^2}{2m})\}d\alpha, \quad (19)$$

which give (for $E<0$)

$$R=(-1)^{n_1+n_2+n'_1+n'_2} [C(n_1 n'_1 \ell_1)C(n_2 n'_2 \ell_2)]^{1/2} (\frac{2}{\hbar\omega}) \times$$

$$\times \sum_{\nu=0}^{n_1+n_2+n'_1+n'_2} (-1)^\nu \{\sum_{S=0}^{n_1+n'_1} (2\ell_1+2S+1)!!(2\ell_2+2\nu-2S+1)!! \times$$

$$\times \sum_{\mu=0}^{n_1} a_\mu(n_1 n'_1 \ell_1, S) \sum_{\mu'=0}^{n_2} a_{\mu'}(n_2 n'_2 \ell_2, \nu-S)\} I_{\ell_1+\ell_2+\nu+3}(\frac{2|E|}{\hbar\omega}), \quad (20)$$

$$C(nn'\ell) = n!n'!(2\ell+2n+1)!!(2\ell+2n'+1)!!/2^{n+n'}, \quad (21)$$

$$a_\mu(nn'\ell, S) = \{\mu!(n-\mu)!(n'+\mu-S)!(S-\mu)! \times$$

$$\times(2\ell+2\mu+1)!!(2\ell+2S-2\mu+1)!!\}^{-1}, \quad (22)$$

$$I_n(\beta) = \frac{1}{(n-1)!}[\sum_{k=1}^{n-1}(k-1)!(-\beta)^{n-k-1} +$$

$$+(-\beta)^{n-1}\exp(\beta)[-Ei(-\beta)]], \quad (23)$$

$$-Ei(-\beta) = \int_\beta^\infty \exp\{-t\}/t\,dt. \quad (24)$$

Accordingly, the evaluation of the double integrals (18) is reduced to the calculation of the algebraic expression (20)-(23) and the one dimensional integral $Ei(-\beta)$.

The matrix elements of the interaction $V(r_1,r_2)$ are most easily calculated in the coordinate representation and in the present work of the programme of ref. /6/ was used for this aim.

It is obvious from the representation given above, that the wave functions of the present approach are immediately obtained in the momentum space (for the sake of simplicity, we here leave out the summation over configurations):

$$\langle \bar{k}_1 \bar{k}_2 | \psi_{JM} \rangle = G_0(E)[\langle \bar{k}_1 | j_1 m_1 \rangle \langle \bar{k}_2 | j_2 m_2 \rangle]^j_m. \quad (25)$$

Making a double Fourier-transformation and reasoning in a way analogous to the deduction of formula (20), we obtain

$$\langle \bar{r}_1, \bar{r}_2 | \psi_{JM} \rangle = [Y^{m_1}_{\ell_1 j_1}(\hat{r}_1) Y^{m_2}_{\ell_2 j_2}(\hat{r}_2)]^j_m \times I_{n_1\ell_1 n_2\ell_2}(r_1,r_2,E), \quad (26)$$

$$I_{n_1\ell_1 n_2\ell_2}(r_1,r_2,E) = \int_0^\infty d\alpha \exp\{-|E|\alpha\} f_{n_1\ell_1}(r_1\alpha) f_{n_2\ell_2}(r_2\alpha), \quad (27)$$

$$f_{n\ell}(r\alpha) = \sqrt{\frac{1}{\sqrt{\pi}} \frac{2^{n+\ell+2}}{n!(2n+2\ell+1)!!} \frac{1}{b^{3/2}} (\frac{r}{b})^\ell \frac{(1-\hbar\omega\alpha)^n}{(1+\hbar\omega\alpha)^{n+\ell+3/2}}} \times$$

$$\times L_n^{\ell+1/2}(\frac{1}{1-(\hbar\omega\alpha)^2}(\frac{r}{b})^2) \exp\{-\frac{1}{2(1+\hbar\omega\alpha)}(\frac{r}{b})^2\}. \quad (28)$$

To normalize the wave functions we must sum a large number of double integrals, but it can also be done in a simpler way. The normalization integral is equal to

$$\langle\psi_1|\psi_1\rangle = \sum_{\substack{\mu\nu\\ij}} \langle\mu|\frac{1}{E-H_0}\cdot\frac{1}{E-H_0}|i\rangle V_{\mu\nu} C_\nu V_{ij} C_j = \tag{29}$$

$$= \sum_{\substack{\mu\nu\\ijm}} \langle\mu|\frac{1}{E-H_0}|m\rangle\langle m|\frac{1}{E-H_0}|i\rangle V_{\mu\nu} C_\nu V_{ij} C_j . \tag{30}$$

If the sum over m runs to ∞, the equality (30) is exact, but in practice, the sum must be cut off. Then, by means of equation (6) we obtain

$$\langle\psi_1|\psi_1\rangle = \sum_m C_m^2 . \tag{31}$$

This relation is an approximate one, the error contained in it depends on the number of configurations N, and numerical calculations have shown, that for $N \geq 30$ this error is $\leq 1\%$.

A more exact formula for the normalization integral can be obtained by using the identity

$$\frac{1}{x^2} = -\frac{d}{dx}\frac{1}{x},$$

which gives

$$\langle\psi_1|\psi_1\rangle = -\frac{\partial}{\partial E}\sum_{\substack{\mu\nu\\ij}} \langle\mu|\frac{1}{E-H_0}|i\rangle V_{\mu\nu} C_\nu V_{ij} C_j . \tag{32}$$

It is clear from (32) that the normalization integral can be calculated with the same degree of exactness as the coefficients C_ν.

NUMERICAL RESULTS

a) The Single-Particle States

The Revai method described here, namely the separable expansion of the potential (MR) was first applied to a simpler problem: the determination of single-particle states in a Saxon-Woods well [5]. Maybe it will be useful to show how it works in this case as compared to the usual

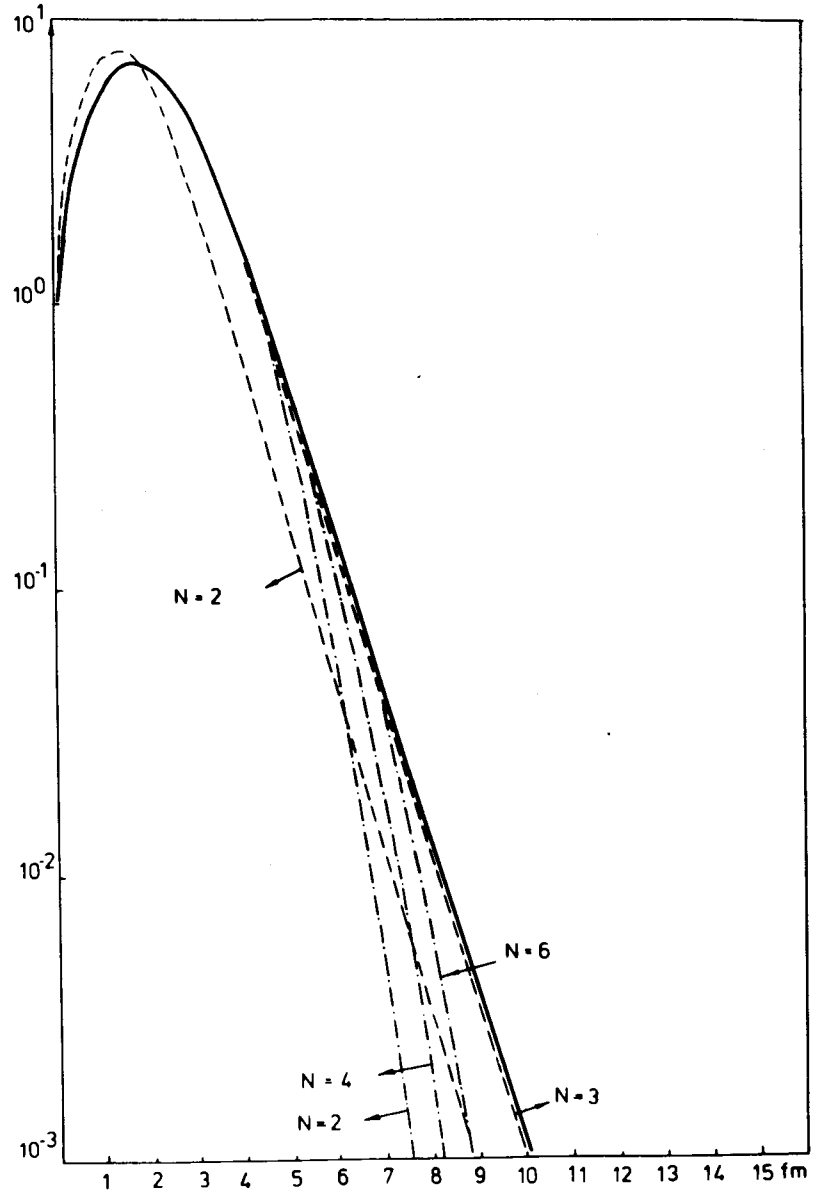

Fig. 1. Wave function of the 1s state of ^{17}O (—— exact, - - - - MR, -·-·- MD).

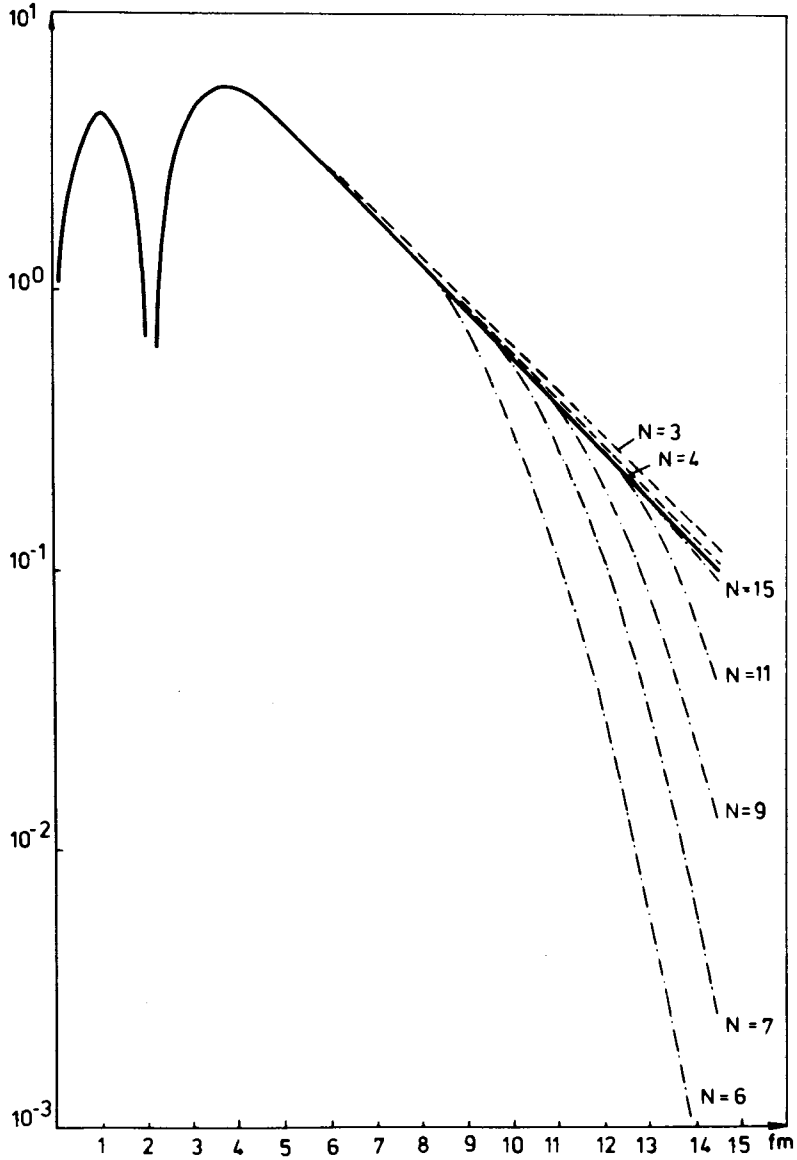

Fig. 2. Wave function of the 2s state of ^{17}O (—— exact, - - - - MR, -·-·- MD).

diagonalization method (MD). The potential was chosen to represent the ^{16}O average well: $V_0 = 51.3$ *MeV*, a = = .6289 *fm*, $R_0 = 3.1246$ *fm* (= 1.24 *fm* $\cdot 16^{1/3}$).

We now compare our results obtained with the two methods mentioned above as functions of the number of terms, N, in the expansion with the exact ones, obtained by numerical integration. The results are expected to depend strongly on the parameter b. In MD this is actually so, the optimal values of b are very different for the strongly bound 1s state and the loosely bound 2s state (1.55 *fm* and 2.25 *fm*, respectively). In MR the optimal b's are nearly identical (1.35 *fm*). In the calculations it is usually wanted, that the approximate wave functions are orthogonal but this is only the case, when they are calculated with the same b. We must therefore choose a common b for the 1s and 2s state also in MD, and we choose b = 1.90 *fm*. The results of this calculation are given in *Tables 1* and *2*.

Table 1

Results for the 1s state. The exact binding energy is $E_{1s} = 31.1002$ *MeV*. The non-filled columns mean, that the values do not change any more with

N	MD b=1.55 fm	MD b=1.90 fm	MR b=1.35 fm
	E_{1s}, MeV	E_{1s}, MeV	E_{1s}, MeV
1	31.0788	31.0476	31.3456
2	31.0791	31.0861	31.1379
3	31.0997	31.0911	31.0955
4	31.0999	31.0968	31.0986
5	31.1000	31.0996	31.1001
6	31.1002	31.1001	31.1002
7		31.1001	
8		31.1001	
9		31.1001	
10		31.1002	

Table 2

Results for the 2s state. The exact binding energy is: $E_{2s} = 3.2084$ *MeV*

N	MD b=2.25 fm	MD b=1.90 fm	MR b=1.35 fm
	E_{2s}, MeV	E_{2s}, MeV	E_{2s}, MeV
1	.9968	2.1578	-
2	1.4268	2.1759	4.1457
3	2.9681	3.0258	3.4128
4	3.0620	3.0909	3.1632
5	3.1949	3.1301	3.2055
6	3.1949	3.1772	3.2123
7	3.1990	3.1834	3.2073
8	3.2039	3.1968	3.2080
9	3.2040	3.2001	3.2083
10	3.2072	3.2033	3.2083
11	3.2072	3.2052	3.2084
12	3.2082	3.2061	
13	3.2082	3.2070	
14	3.2083	3.2074	
15	3.2084	3.2078	

Figures 1 and *2* show the wave function calculated by MR and MD for different N-values, and the optimal b-value. The difference between the two methods is clearly seen, the Revai method gives more correct wave functions, particularly for the weakly bound state. Further even when the two methods give equally precise energy values, the wave functions, calculated with MR are more exact in the asymptotic region, than those of MD.

b) The 0^+ State of ^{18}O

As a mean field of the oxygen nucleus we shall again use the Woods-Saxon potential with the parameters given in *Table 3*. The spin-orbital term was chosen to be

$V_{s.o.} = V_0 \kappa \frac{1}{r} \frac{d}{dr}[1+\exp(\frac{r-R}{a})]^{-1} (\vec{\ell}\vec{\sigma})$. The residual interaction we take to be

$$V(r_{12}) = V_{res} \frac{\mu}{r} \exp\{-\frac{r}{\mu}\}$$

with $V_{res} = 20.5$ *MeV*, $\mu = 1.4$ *fm*.

It is obvious, that equation (1) cannot be solved exactly with such a potential energy. We can, however, compare the MR and MD solutions with $V(r_{12})=0$ with the corresponding exact solutions. In *Tables 4* and *5* this is done for the eigenvalues of the states $(2s,2s)^{0+}$ and $(1d\ 5/2,1d\ 5/2)^{0+}$ for different values of N and b. *Figure 3* shows the functions $R_{2s}(r) = \langle 2s|(2s,2s)^{0+}\rangle$ and it is seen, as expected, that the asymptotic form of the functions is more correct in MR than in MD.

In the case of $V(r_{12}) \neq 0$ the configuration space was limited to $\ell = 0., 2.,$, $j = 1/2, 3/2, 5/2,$ and energy eigenvalues were calculated for a number of N-values, as given in *Table 6*. The logarithm of the wave function $\ln\psi(\rho,\Omega)$ for $\Omega = (0,0,\frac{\pi}{4})$ is seen in *fig. 4*. It obviously shows the correct "three-particle" asymptotic form. The difference between the wave functions calculated with the MR and MD is growing with ρ, and for $\rho \sim 14$ the MR function is about 10^6 times larger than the MD one.

It is seen that the method suggested here gives a convergence in the energy calculation for the ground state ^{18}O which is at least as rapid as that of the MD. But the MR gives the correct asymptotic form of the wave functions even for a small number of basis functions, whereas this is with MD obtained only at the expense of enlarging the basis space to an extreme degree even for moderate values of r_1, r_2 or ρ.

We have here considered the energy E as eigenvalue. This was specially done in order to compare our method with the standard diagonalization method. Then we had to calculate many matrix elements $\langle i|G_0(E)|j\rangle$ for different E values as long as the determinant (7)

Table 3

Parameters for potentials

V_0 (MeV)	κ (fm^2)	a (fm)	r_0 (fm)
53.41	.216	.65	1.24

Table 4

Results for the $(1d_{5/2}, 1d_{5/2})^{0+}$ state. The exact energy is E = 8.1533 *MeV*

β (fm)		N=3	N=6	N=10	N=15	N=21
1.387	MD	5.2159	6.6208	7.4558	7.7914	7.9442
	MR	7.9329	7.3368	7.9343	8.0159	8.0594
1.687	MD	7.1642	7.7868	8.0424	8.0743	8.1268
	MR	7.2192	8.0289	8.1615	8.0915	8.1583
1.987	MD	6.6523	8.0987	8.1037	8.1311	8.1492
	MR	6.9818	8.5417	8.1057	8.1430	8.1581
2.287	MD	4.4633	7.3647	7.8817	8.1270	8.1459
	MR		8.1153	8.0531	8.2154	8.1536

Table 5

Results for the $(2s\ 2s)^{0+}$ state. The exact energy is E = 6.472 *MeV*

β (fm)		N=6	N=10	N=15	N=21
1.387	MD	-	2.2869	4.1429	5.0571
	MR	4.0088	4.5476	5.6957	5.9686
1.687	MD	3.7544	5.1444	5.8586	6.0537
	MR	4.5114	6.0298	6.4007	6.1766
1.987	MD	4.1255	6.1815	6.2264	6.3264
	MR	4.2385	7.0822	6.2556	6.3967
2.287	MD	2.6883	5.9127	6.1187	6.4226
	MR	3.3238	7.2237	6.2540	6.6056

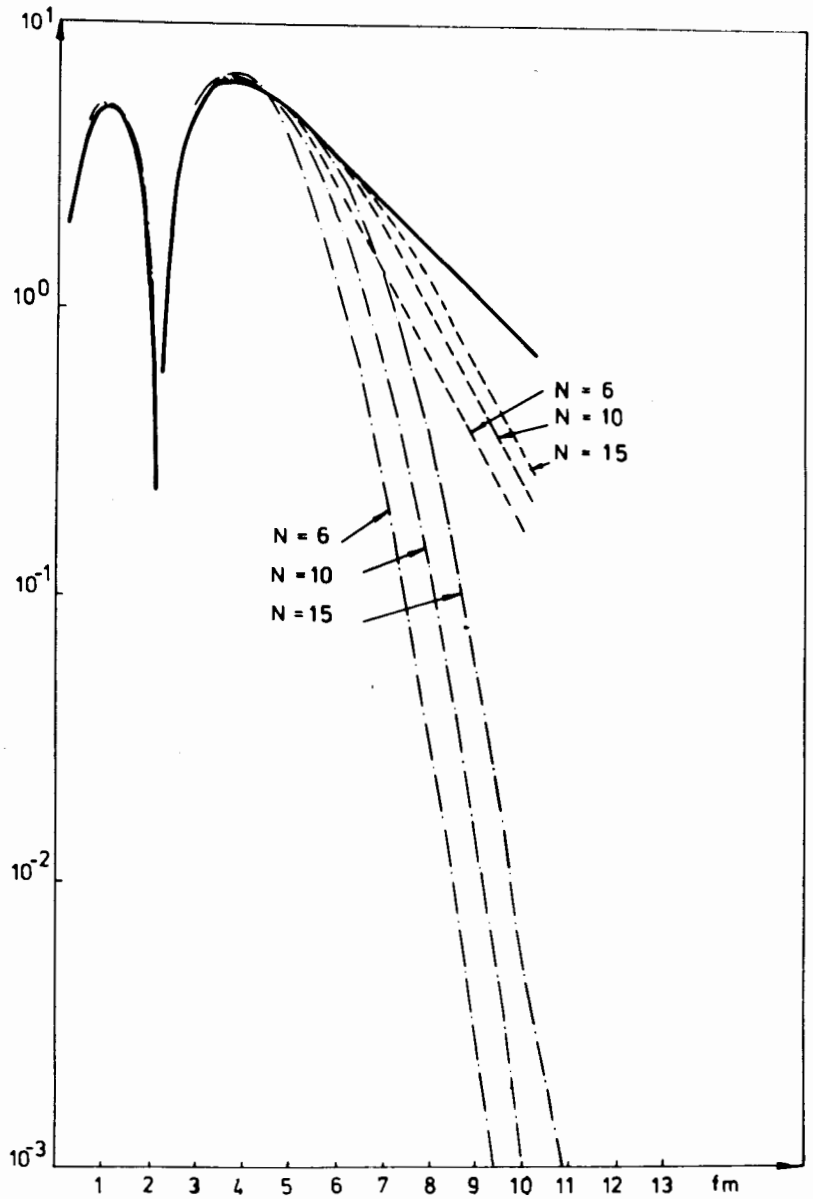

Fig. 3. Overlap integral $<R_{2s}(\bar{r}_1)|\psi(\bar{r}_1,\bar{r}_2)>$ *(see text). (—— exact, - - - - MR, -·-·-· MD).*

is different from zero within the given precision. At this point, the MR differs from MD by requiring long calculation time.

If, on the other hand, we want to calculate the cross sections for direct reaction processes, where E can be taken from the experiment it is more natural to consider λ (the depth of the mean field) or γ (the coupling constant of the residual interaction) as eigenvalue. Then the asymptotic form of the wave function will be correct for

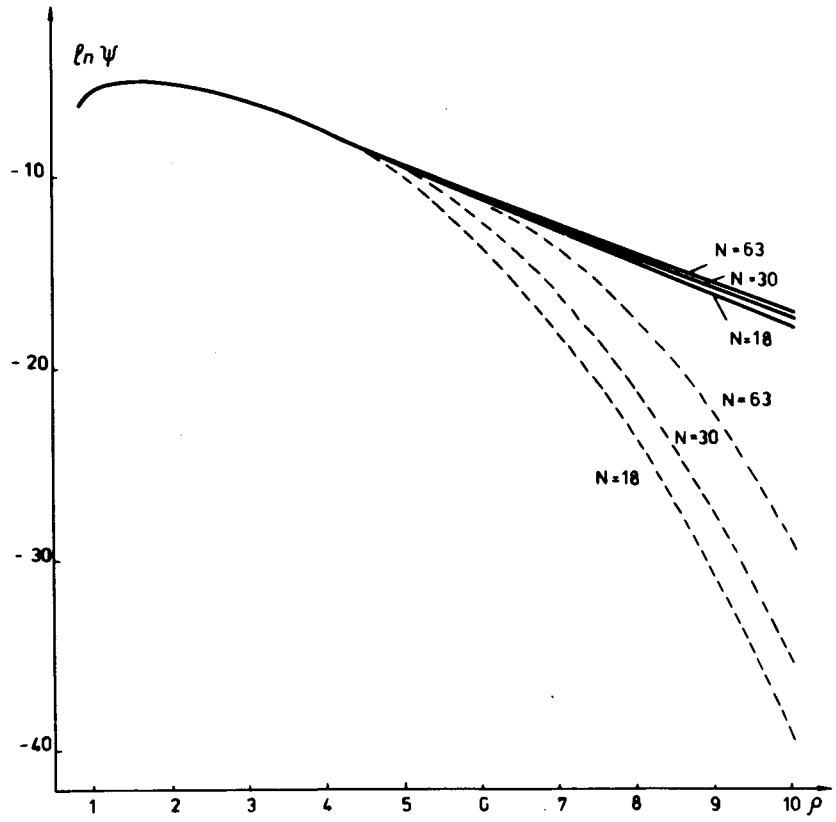

Fig. 4. Wave function $\psi(\rho,0,0,\frac{\pi}{4})$ *of the ground state of* ^{18}O *(——— MR, - - - MD).*

Table 6

Results for the 0^+ ground state (b = 1.678 *fm*)

	N=9	N=18	N=30	N=45	N=63
MD	-9.5268	-10.0182	-10.2329	-10.2549	-10.2938
MR	-9.3887	-10.1956	-10.3262	-10.2674	-10.3142

any choice of the oscillator basis space; only the asymptotic normalization will depend on this choice. In this way MR can be said to be used to calculate the vertex constant which enters into the diagram method of calculation of nuclear reaction cross sections /7/.

In this case the matrix elements $\langle i|G_0(E)|j\rangle$ shall only be calculated one time for the experimental energy value $E_0 = E_{exp}$ and the eigenvalue of λ or γ can be found by usual matrix diagonalization methods. Then MR will need approximately the same calculation time as MD, but it still retains the advantages over this method, which have been mentioned above.

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APPENDIX

The wave function in the coordinate space (ρ,Ω).

According to Eq. (5) the momentum space wave function can be written as

$$\langle \bar{k}_1, \bar{k}_2 | JM\rangle = \frac{1}{k_1^2 + k_2^2 + c^2} \sum_{\mu_1\mu_2} \langle \bar{k}_1, \bar{k}_2 | \mu_1\mu_2; JM\rangle C_{\mu_1\mu_2} \quad (A.1)$$

where $|\mu_1\mu_2; JM\rangle$ is a product of two single-particle oscillator states coupled to total angular momentum J, c is related to the energy eigenvalue: $c = -\frac{2mE}{\hbar^2}$

and the coefficients $C_{\mu_1\mu_2}$ are the solutions of the linear system (6).

The transformation of (A.1) into the coordinate space can be done conveniently in two steps. First, introducing the hyperspherical variables (k,Ω) instead of the two vectors $(\bar{k}_1,\bar{k}_2)$ by

$$k^2 = k_1^2 + k_2^2$$

$$\Omega = (\omega_1, \omega_2, \alpha = \mathrm{arctg}\frac{k_2}{k_1}), \qquad \text{(A.2)}$$

ω_i being the three-dimensional solid angle of $\bar{k}_i$, the product state $|\mu_1\mu_2; JM\rangle$ can be expressed /8/ as a superposition of states of a six-dimensional harmonic oscillator having the same number of oscillator quanta:

$$|n_1\ell_1 j_1, n_2\ell_2 j_2; JM\rangle = \sum_{\substack{N,n \\ N+n=n_1+n_2}} |Nn\,\ell_1 j_1\,\ell_2 j_2; JM\rangle \langle Nn|n_1 n_2\rangle_{\ell_1\ell_2}, \qquad \text{(A.3)}$$

where the following notation was used:

$$\langle k\Omega|Nn\ell_1 j_1\,\ell_2 j_2; JM\rangle = \left[\frac{2N!}{(N+K+2)!}\right]^{1/2} k^K \exp\{-\frac{1}{2}k^2\} \times$$

$$\times L_n^{K+2}(k^2)\, Y_K^{\ell_1 j_1 \ell_2 j_2 JM}(\Omega), \qquad \text{(A.4)}$$

$$K = 2n + \ell_1 + \ell_2,$$

L_n^{K+2} is the usual Laguerre-polynomial, and $Y_K(\Omega)$ is a six-dimensional hyperspherical function:

$$Y_K^{\ell_1 j_1 \ell_2 j_2 JM}(\Omega) = \left[\frac{2\cdot(K+2)\,n!(n+\ell_1+\ell_2+1)!}{\Gamma(n+\ell_1+3/2)\cdot\Gamma(n+\ell_2+3/2)}\right]^{1/2} (\cos\alpha)^{\ell_1} (\sin\alpha)^{\ell_2} \times$$

$$P_n^{\ell_2+1/2,\ell_1+1/2}(\cos 2\alpha)\left[Y_{\ell_1}^{j_1}(\omega_1)\cdot Y_{\ell_2}^{j_2}(\omega_2)\right]^{JM}. \qquad \text{(A.5)}$$

The restriction $N+n=n_1+n_2$ in the sum (A.3) expresses the conservation of the number of oscillator quanta. A detailed description of the transformation (A.3) together with the discussion of the properties of the coefficients $\langle Nn|n_1 n_2\rangle_{\ell_1\ell_2}$ can be found in /8/.

By using (A.3) the wave function (A.1) can be written as

$$\langle \bar{k}_1, \bar{k}_2|JM\rangle = \langle k\Omega|JM\rangle =$$

$$= \frac{1}{k^2+c^2} \sum_{\substack{Nn \\ \ell_1 j_1 \\ \ell_2 j_2}} \langle k\Omega|Nn\ell_1 j_1\,\ell_2 j_2; JM\rangle \tilde{C}_{Nn\ell_1 j_1 \ell_2 j_2} \qquad \text{(A.6)}$$

with

$$\tilde{C}_{Nn\ell_1 j_1 \ell_2 j_2} = \sum_{\substack{n_1 n_2 \\ n_1+n_2=N+n}} C_{n_1\ell_1 j_1 n_2 \ell_2 j_2} \langle Nn|n_1 n_2\rangle_{\ell_1\ell_2}.$$

The double Fourier transformation leading to the coordinate representation of (A.6) can be now easily performed using the expansion of the six-dimensional plane wave $\exp\{i(\bar{k}_1\bar{r}_1 + \bar{k}_2\bar{r}_2)\}$ in terms of the six-dimensional (hyper) spherical harmonics /9/. We obtain

$$\langle \bar{r}_1, \bar{r}_2|JM\rangle = \langle \rho, \Omega|JM\rangle =$$

$$= \sum_{\substack{Nn \\ \ell_1 j_1 \ell_2 j_2}} F_{NK}(\rho)\, Y_K^{\ell_1 j_1 \ell_2 j_2 JM}(\Omega), \qquad \text{(A.7)}$$

where (ρ,Ω) are the hyperspherical variables (A.2) for the pair of vectors $(\bar{r}_1,\bar{r}_2)$ and

$$F_{NK}(\rho) = \left[\frac{2N!}{(N+K+2)!}\right]^{1/2} (2\pi)^3 \frac{1}{\rho^2} \int_0^\infty \frac{J_{K+2}(k\rho)\exp\{-\frac{1}{2}k^2\} L_n^{\ell+1/2}(k^2)\, k^{K+3}}{k^2+c^2}\, dk. \qquad \text{(A.8)}$$

The asymptotic form of the wave function (A.7) for large ρ can be obtained by using the standard methods for asymptotic estimation of the integral (A.8). This gives

$$F_{NK}(\rho) \underset{\pi\to\infty}{\longrightarrow} a_{NK}\frac{\exp\{-c\rho\}}{\rho^{5/2}} \qquad (A.9)$$

confirming the form (13).

Let us look at the overlap integral of the one-particle wave functions of ^{17}O and the wave function of ^{18}O. For simplicity we restrict ourselves to the lowest term ψ_{1s1s} in ψ. Then we obtain

$$<R_{1s}(\bar{r}_1)|\psi_{1s1s}(\bar{r}_1,\bar{r}_2)> \sim \frac{1}{r_2}\int_0^\infty \frac{k_1^2\exp\{-k_1^2b^2\}}{k_1^2+d^2}dk_1 \times$$

$$\times \int_0^\infty \frac{k_2\sin(k_2r_2)}{k_1^2+k_2^2+c^2}\exp\{-k_2^2\frac{b^2}{2}\}dk_2 = \qquad (A.10)$$

$$= A\int_0^\infty dx \frac{\exp\{-xc^2-\frac{r_2^2}{4(b^2/2+x)}\}}{(\frac{b^2}{2}+x)^{3/2}}\{\frac{1}{\sqrt{b^2+x}}-d\sqrt{\pi}\exp\{d^2(b^2+x)\}\times$$

$$\times(1-\phi(d\sqrt{b^2+x}))\},$$

where $d^2=-\frac{2mE_1}{\hbar^2}$, E_1 is the one particle separation energy of the state in question in ^{17}O. In deriving (A.10) we have twice used (19). We can use the following representation of the function $\phi(y)$:

$$\phi(y)=1-\frac{1}{\sqrt{\pi}}\frac{\exp\{-y^2\}}{y} \quad \text{for } y\to\infty. \qquad (A.11)$$

and inserting (A.11) into (A.10) we get

$$<R_{1s}(\bar{r}_1)|\psi_{1s1s}(\bar{r}_1,\bar{r}_2)> \approx \frac{\exp\{-cr_2\}}{r_2^{3/2}}, \quad \text{for } r_2\to\infty. \qquad (A.12)$$

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