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A.Săndulescu, I.Şilisteanu

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1. INTRODUCTION

It is well known that the calculation of two particle shell model matrix elements, the spectroscopy factors for transfer reactions with two or more particles transferred, or of the reduced widths of alpha decay is enormously simplified if the two particle wave functions are expressed in terms of the relative and centre-of-mass coordinates of the system.

For single particle wave functions characteristic of an infinite harmonic oscillator well, Talmi [1] and Moshinsky [2] have developed explicit methods for performing the transformation of two particle wave functions from individual coordinates to relative and centre-of-mass ones.

For two-particle wave functions characteristic of a finite potential well, i.e., Woods-Saxon potentials, Bayman and Kallio [3] have given a numerical procedure for performing this transformation. This method, however, was restricted to the zero relative angular momentum of two-nucleon wave functions. Recently [4] this restriction has been removed.

In the present paper a new method is developed. In section 2, by transforming analytically the angular parts of two-particle wave functions and by expanding the corresponding radial parts around the centre-of-mass of the two-particle system, explicit expressions of two-particle wave functions in relative and center-of-mass coordinates are obtained. In section 3, the overlap integrals for two particles are studied. It is shown that for harmonic oscillator single particle wave functions

our procedure is quite convergent and leads to values identical with those obtained by applying the Talmi-Moshinsky procedure. Also a good convergence of the procedure is indicated by the overlap integrals with Woods-Saxon single particle wave functions. In our procedure the computing time is shorter than that needed for other procedures [2-4].

This method can also be used in "finite range" calculations of transfer reactions with many particles transferred or in the Hartree-Fock calculations of atomic nuclei.

2. *RELATIVE AND CENTRE OF MASS WAVE FUNCTIONS*

The normalized wave function for two particles situated in a central potential V(r) is given by

$$\Psi_{n_1\ell_1 n_2\ell_2\lambda\mu}(\vec{r}_1,\vec{r}_2)=[2(1+\delta_{n_1n_2}\delta_{\ell_1\ell_2})]^{-1/2}\{[\Psi_{n_1\ell_1}(\vec{r}_1),\Psi_{n_2\ell_2}(\vec{r}_2)]_{\lambda\mu}+$$

$$+[\Psi_{n_1\ell_1}(\vec{r}_2),\Psi_{n_2\ell_2}(\vec{r}_1)]_{\lambda\mu}\}, \qquad (1)$$

where

$$\Psi_{n\ell m}(\vec{r}_i)=\mathcal{R}_{n\ell}(r_i)Y_{\ell m}(\hat{r}_i) \qquad (2)$$

are single particle states derived from the Schrödinger equation

$$[-\frac{h^2}{2m}\Delta+V(r)-E]\Psi_{n\ell m}(\vec{r})=0. \qquad (3)$$

For single particle harmonic oscillator potentials the wave function (1) can be easily expressed in terms of the relative $\vec{r}_{12}=\sqrt{2}\vec{r}$ and centre-of-mass coordinates $\vec{R}_c=\frac{1}{\sqrt{2}}\vec{R}$,

where $\vec{r}=\frac{1}{\sqrt{2}}(\vec{r}_1-\vec{r}_2)$ and $\vec{R}=\frac{1}{\sqrt{2}}(\vec{r}_1+\vec{r}_2)$, (4)

using the Talmi-Moshynsky transformation brackets

$$[\Psi_{n_1\ell_1}(\vec{r}_1),\Psi_{n_2\ell_2}(\vec{r}_2)]_{\lambda\mu}=\sum_{n\ell NL}<n\ell,NL,\lambda|n_1\ell_1,n_2\ell_2,\lambda>\times$$

$$\times[\Psi_{n\ell}(\vec{r}),\Psi_{NL}(\vec{R})]_{\lambda\mu}, \qquad (5)$$

under the conditions

$$2n_1+\ell_1+2n_2+\ell_2=2n+\ell+2N+L,$$

$$(-1)^{\ell_1+\ell_2}=(-1)^{\ell+L}. \qquad (6)$$

We should like to stress that the above transformation brackets can be defined only for Hamiltonians which are separable after transformation (4).

Below, a new method is developed by expanding the single particle states around the centre-of-mass of the system. In this way the wave functions (1) can be written directly in terms of the initial wave functions and their derivatives in the new coordinates (5).

Indeed, let us write (1) in the form

$$[\Psi_{n_1\ell_1}(\vec{r}),\Psi_{n_2\ell_2}(\vec{r})]_{\lambda\mu}=\tilde{\mathcal{R}}_{n_1\ell_1}(r_1)\tilde{\mathcal{R}}_{n_2\ell_2}(r_2)[\mathcal{M}_{\ell_1}(\vec{r}_1),\mathcal{M}_{\ell_2}(\vec{r}_2)]_{\lambda\mu}, \qquad (7)$$

where

$$\mathcal{M}_{\ell_i m_i}(\vec{r}_i)=r_i^{\ell_i}Y_{\ell_i m_i}(\hat{r}_i) \qquad (8)$$

is a multipolar field and

$$\tilde{\mathcal{R}}_{n_i\ell_i}(r_i)=\mathcal{R}_{n_i\ell_i}(r_i)r_i^{-\ell_i} \qquad (9)$$

is the modified radial part of the wave function (2).

Thus, due to the fact that the multipoles in the old and new coordinates are solutions of the Laplace equation and that the first multipoles can be written in terms of the products of the second ones,

$$\mathcal{M}_{\ell_i m_i}(\vec{r}_i)=\sum_{\ell'\ell''}\delta_{\ell,\ell'+\ell''}\,A(\ell',\ell'',\ell)\left(\frac{r}{\sqrt{2}}\right)^{\ell'}\left(\frac{R}{\sqrt{2}}\right)^{\ell''}[Y_{\ell'}(\hat{r}),Y_{\ell''}(\hat{R})]_{\lambda\mu}, \tag{10}$$

where

$$A(\ell',\ell'',\ell)=(-)^{\ell''}[4\pi(2\ell+1)!/(2\ell'+1)!(2\ell''+1)!]^{1/2}, \tag{11}$$

the multipolar part of the wave function (7), becomes

$$[\mathcal{M}_{\ell_1}(\vec{r}_1),\mathcal{M}_{\ell_2}(\vec{r}_2)]_{\lambda\mu}=\left(\frac{R^2}{2}\right)^{\frac{\ell_1+\ell_2}{2}}\sum_{\ell,L,s}Q_{\ell_1\ell_2\lambda}(\ell,L,s)\times$$

$$\times\left(\frac{r}{R}\right)^{s}[Y_\ell(\hat{r}),Y_L(\hat{R})]_{\lambda\mu}, \tag{12}$$

$$Q_{\ell_1\ell_2\lambda}(\ell,L,s)=\sum_{\ell'}(-)^{\ell'}A(\ell_1-\ell',\ell',\ell_1)A(\ell_2+\ell'-s,s-\ell',\ell_2)\times$$

$$\times B(\ell',s-\ell',\ell)(B(\ell_1-\ell',\ell_2+\ell'-s,L)\hat{\ell}_1\hat{\ell}_2\hat{\ell}\,\hat{L}\begin{Bmatrix}\ell' & s-\ell' & \ell\\ \ell_1-\ell' & \ell_2+\ell'-s & L\\ \ell_1 & \ell_2 & \lambda\end{Bmatrix} \tag{13}$$

where

$$B(\ell',\ell'',\ell)=[(2\ell'+1)(2\ell''+1)/4\pi(2\ell+1)]^{1/2}\,C^{\ell'\ell''\ell}_{000}. \tag{14}$$

On the other hand, by writing explicitly $\vec{r}_1$ and $\vec{r}_2$ in terms of r, R and $\cos\theta=(\vec{R}\cdot\vec{r})/R\cdot r$, expanding (10) around R in powers of (r/R) and $\cos\theta$ and replacing the powers of $\cos\theta$ in terms of the corresponding spherical harmonics for each coordinate[5]

$$\cos^q\theta=\sum_{sm}p(q,s)Y_{sm}(\hat{R})Y_{sm}(\hat{r}), \tag{15}$$

where

$$p(q,s)=4\pi\,\frac{(2s+1)^{1/2(s-q-2)}}{((q-s)/2)!(q+s+1)!!}, \tag{16}$$

we obtain

$$\tilde{\mathcal{R}}_{n_1\ell_1}(r_1)\tilde{\mathcal{R}}_{n_2\ell_2}(r_2)=R_c^{-\ell_1-\ell_2}\mathcal{R}_{n_1\ell_1}(R_c)\,\mathcal{R}_{n_2\ell_2}(R_c)\times \tag{17}$$

$$\times\sum_{t,q}P^{t,q}_{n_1\ell_1,n_2\ell_2}(R_c)\left(\frac{r}{R}\right)^t\sum_s(-)^s\hat{s}\,p(q,s)[Y_s(\hat{R}),Y_s(\hat{r})]_{00}.$$

Here the corresponding coefficients of powers $(r/R)^t$ and $\cos^q\theta$ in terms of $\tilde{\mathcal{R}}_{n_i\ell_i}(R_c)$ and their derivatives $\tilde{\mathcal{R}}^{(n)}_{n_i\ell_i}(R_c)$ in the centre-of-mass R_c are denoted by

$$P^{tq}_{n_1\ell_1,n_2\ell_2}(R_c)=(\tilde{\mathcal{R}}_{n_1\ell_1}(R_c)\tilde{\mathcal{R}}_{n_2\ell_2}(R_c))^{-1}\times \tag{18}$$

$$\times\sum_{n\geq k}\sum_{n'\geq k'}(-1)^{k'}2^{k+k'}\binom{n}{k}\binom{n'}{k'}\tilde{\mathcal{R}}^{(n)}_{n_1\ell_1}(R_c)\,\tilde{\mathcal{R}}^{(n')}_{n_2\ell_2}(R_c),$$

where $t=2(n+n')-q$ $\qquad n'+n'\geq q=k+k'$.

For harmonic oscillator potentials the derivatives can be obtained analytically. For Woods-Saxon potentials these derivatives must be computed numerically[6], the higher orders derivatives being reduced to the first orders by using the Schrödinger equation (3).

Finally, by combining the multipolar parts (12) and the modified radial part (17) of the wave functions (7) and reintroducing the full wave functions in the centre-of-mass we obtain

$$[\Psi_{n_1\ell_1}(\vec{r}_1),\Psi_{n_2\ell_2}(\vec{r}_2)]_{\lambda\mu}=\mathcal{R}_{n_1\ell_1}(R_c)\mathcal{R}_{n_2\ell_2}(R_c)\sum_{t,q,s}P^{tq}_{n_1\ell_1,n_2\ell_2}(R_c)\times$$

$$\times(r/R)^{t+s}\,\frac{2s+1}{4\pi}p(q,s)\Sigma(-1)^L\hat{\ell}\hat{L}\,Q_{\ell_1\ell_2\lambda}(\ell,L,s)\times$$

$$\times \sum_{\ell' L'} (-1)^{L'} \begin{Bmatrix} \ell' & L' & \lambda \\ L & \ell & s \end{Bmatrix} C^{sLL'}_{000} \, C^{s\ell\ell'}_{000} \, [Y_{L'}(\hat{R}), Y_{\ell'}(\hat{r})]_{\lambda\mu}. \tag{19}$$

3. TWO PARTICLE OVERLAP INTEGRALS

The overlap integrals for the emission or transfer of two particles coupled to angular momentum λ are defined by

$$I_{n_1\ell_1, n_2\ell_2, \lambda}(R) = \int \Psi_{n_1\ell_1 n_2\ell_2 \lambda\mu}(\vec{r}_1, \vec{r}_2) Y_{\lambda\mu}(\hat{R}) \Phi_\alpha(\vec{r}) \, d\Omega_R d\vec{r}, \tag{20}$$

where $Y_{\lambda\mu}(\hat{R})$ is a spherical harmonic and $\Phi_\alpha(\vec{r})$ is the intrinsic wave function of the two-particle system assumed to have an intrinsic angular momentum equal to zero and a Gaussian-type function for the radial part

$$\Phi_\alpha(\vec{r}) = N_\alpha \exp\left(-\frac{\beta r^2}{2}\right) Y_{00}(\hat{r}) \tag{21}$$

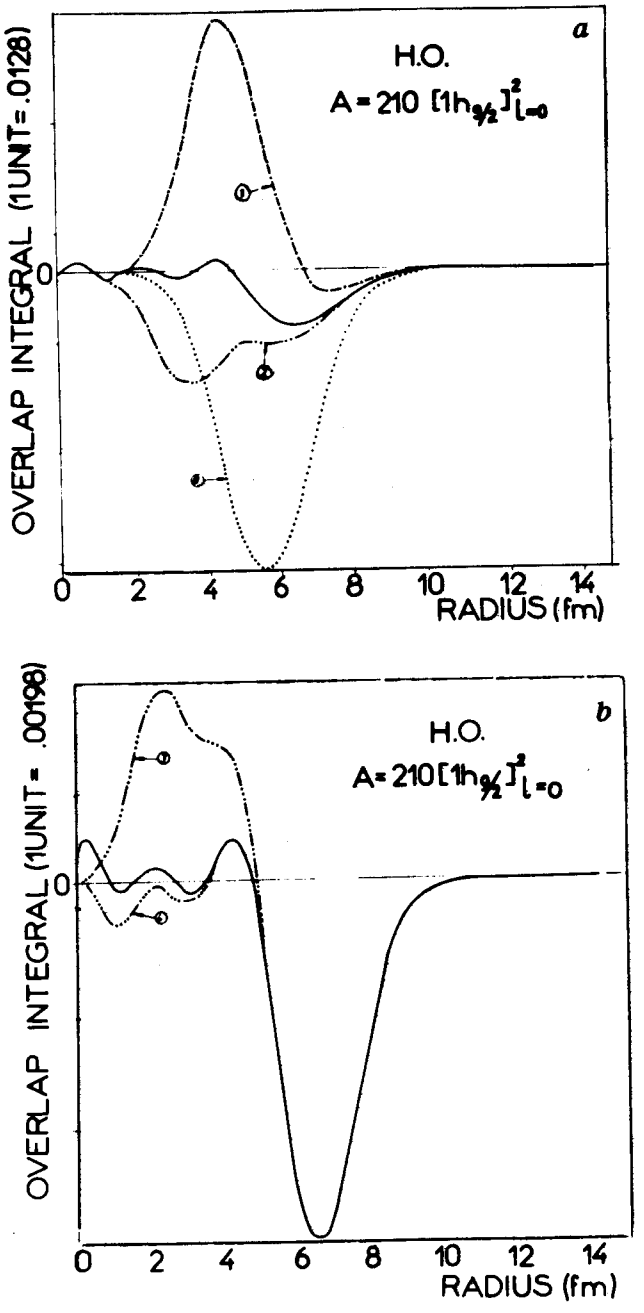
with the parameter $\beta = 0.434\ fm^{-2}$ correspondong to the size of the alpha particle.

Using expressions (19) and (21) in eq. (20), we obtain

$$I_{n_1\ell_1, n_2\ell_2, \lambda}(R_c) = 2N_\alpha [2(1+\delta_{n_1 n_2}\delta_{\ell_1\ell_2})]^{-1/2} \mathcal{R}_{n_1\ell_1}(R_c) \mathcal{R}_{n_2\ell_2}(R_c) \times$$

$$\times \sum_{tqs} P^{tq}_{n_1\ell_1, n_2\ell_2}(R_c) p(q,s) \sum_L \frac{\hat{s}\hat{L}}{4\pi\lambda} C^{sL\lambda}_{000} Q(s, L, s) J_{t+s}(R_c), \tag{22}$$

Fig. 1. The overlap integral, for harmonic oscillator wave function and the configuration $(1h_{9/2})^2$ $\ell = 0$ *as a function of radius for the zero-range or point approximation* $q = t+s = 0$ (...), *zero range plus first* $q=2$ (-.-.), *second* $q=4$ (-..-), *third* $q=6$ (-...-), *fourth* $q=8$ (-.....-) *order corrections and the exact values* (——).



where

$$J_k(R_c) = R_c^{-k} \int_0^\infty r^{k+2} \exp(-\beta r^2/2)\, dr . \qquad (23)$$

One of the most usual approximations for the integral (20) is the so-called "point approximation", which consists in neglecting the finite size of the transferred system in the single particle wave functions

$$\Psi_{n_i \ell_i m_i}(\vec{r}_i) \simeq \Psi_{n_i \ell_i m_i}(\vec{R}_c).$$

This approximation is the first term of eq. (22) for $t = q = s = 0$ and $P^{00}_{n_1\ell_1, n_2\ell_2}(R_c) = 1$.

For harmonic oscillator wave functions, by using (5) in expression (20) and integrating the latter, we obtain

$$I_{n_1\ell_1, n_2\ell_2, \lambda}(R_c) = \sum_{nN} < n0, N\lambda, \lambda \mid n_1\ell_1, n_2\ell_2, \lambda > \mathcal{J}_n \mathcal{R}_{N\lambda}(R_c), \qquad (24)$$

where

$$\mathcal{J}_n = \int_0^\infty r^2 \mathcal{R}_{n0}(r) \exp\left(-\frac{\beta r^2}{2}\right) dr . \qquad (25)$$

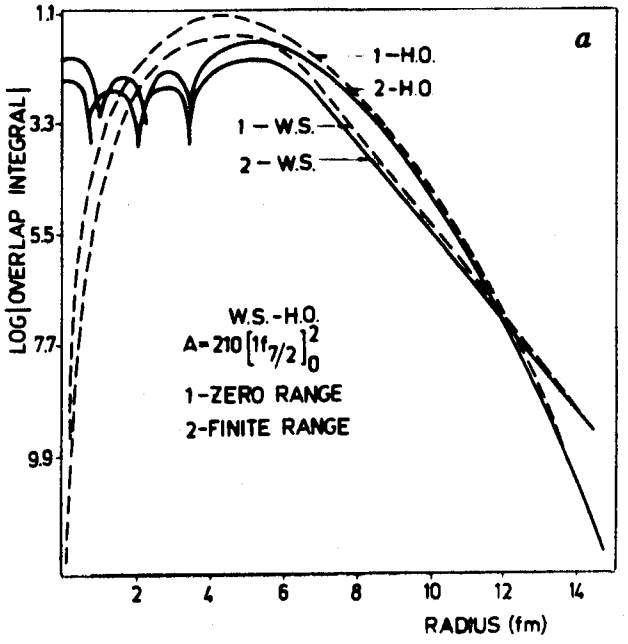
In our procedure, if one takes into account that for harmonic oscillator wave functions the exponential factor of the product of two modified radial parts,

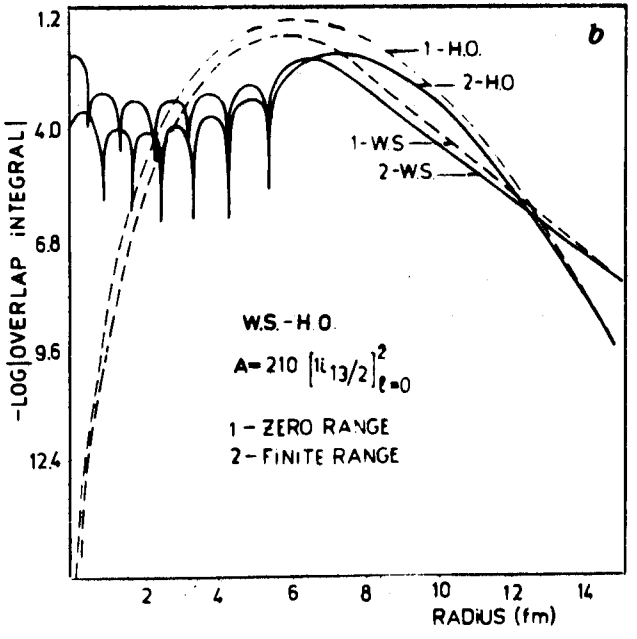
$$\tilde{\mathcal{R}}_{n_1\ell_1}(r_1)\, \tilde{\mathcal{R}}_{n_2\ell_2}(r_2) \sim$$

$$\exp[-\alpha(r^2+R^2)]\, L_{n_1}^{\ell_1+\frac{1}{2}} \left[\frac{\alpha R^2}{2}\left(1+2\frac{r}{R}\cos\theta+\frac{r^2}{R^2}\right)\right] L_{n_2}^{\ell_2+\frac{1}{2}} \times$$

$$\times \left[\frac{\alpha R^2}{2}\left(1-2\frac{r}{R}\cos\theta+\frac{r^2}{R^2}\right)\right], \qquad (26)$$

Fig. 2. The overlap integral, for harmonic oscillator and Woods-Saxon wave functions, for the zero-range or point approximation (- - -) and finite range calculation (——). The configurations $(1f_{7/2})^2\ \ell=0$ *and* $(1i_{13/2})^2\ \ell=0$ *are given in Fig. 2a and Fig. 2b, respectively.*





can be written directly in the new coordinates, we have to expand only the Laquerre polynomials. Thus we obtain a finite number of terms in (18) and (22), similar to the above results, (24), where the number of terms is restricted by (6).

In order to illustrate the convergence of our method, we present on *Fig. 1,* for harmonic oscillator wave functions and the configuration $(1h_{9/2})^2_{\ell=0}$, the overlap integral as a function of radius for different approximations. We can see that the successive finite range corrections to the zero range or point approximation are improving successively the description of the overlap integral starting with larger R-values and giving finally identical results with the Talmi-Moshinsky procedure (24).

For Woods-Saxon or harmonic oscillator single particle wave functions, we are transforming the expansion (18) in a $2N_{max}+\ell_1+\ell_2$ degree polynomial in r/R by fixing the maximum number of the derivatives $N_{max}=n+n'$.

The results for H.O. and W.S. wave functions[7] and configurations $(1f_{7/2})^2$ $\ell=0$ and $(1i_{13/2})^2$ $\ell=0$ for $N^{H.O.}_{max}=0$ and $N^{W.S.}_{max}=10$, respectively, are given in *Fig. 2.* The figures show that the asymptotic behaviours of the overlap integrals for Woods-Saxon and harmonic oscillator wave functions are quite different and that at the surface of the nucleus the first ones are smaller than the second ones.

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