PHYSICAL REVIEW VOLUME 117, NUMBER 1 JANUARY 1, 1960

Harmonic Oscillator Wave Functions in Nuclear Spectroscopy*†

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(Received July 1, 1959)

Pairing energy calculations are generally carried out assuming the nucleon wave functions are those of an harmonic oscillator. The two-body interaction is assumed to be some function of σ_1, σ_2 and $\mathbf{r}_1-\mathbf{r}_2$. Since the coordinates appear only in the form $\mathbf{r}_1-\mathbf{r}_2$, it is convenient to write the two-body wave function in terms of the relative coordinate, $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$, and the center-of-mass coordinate, $2\mathbf{R}=\mathbf{r}_1+\mathbf{r}_2$. The eigenfunction in the new coordinates can be determined by noting that if the two particles are in the same oscillator level, then $\psi(\mathbf{r}_1,\mathbf{r}_2)$, which is an eigenfunction of H_1+H_2, is also an eigenfunction of H_1 alone. Transforming H_1 to relative and center-of-mass coordinates implies that the operator $\mathbf{p}\cdot\mathbf{P}+mk\mathbf{r}\cdot\mathbf{R}$ (where m is the mass of the particle and k is the spring constant of the oscillator) must give zero when operating on the wave function. This condition plus certain requirements arising from the radial form of the oscillator eigenfunctions is sufficient to determine the wave function in the new coordinate system.

INTRODUCTION

SPECTROSCOPIC calculations are generally carried out by expanding the two-body interaction in terms of Legendre polynomials.[1] The angular integrations are then easily performed and the remaining radial integrals can be done either analytically or numerically, depending on their complexity. In nuclear physics a reasonable approximation to the wave functions involved is provided by the harmonic oscillator potential. Talmi[2] has pointed out that for this potential the two-particle wave function $\phi(\mathbf{r}_1)\chi(\mathbf{r}_2)$ can be written as a finite sum of products of oscillator wave functions of the form $\psi(\mathbf{r})\Psi(\mathbf{R})$, where $\mathbf{r}$ is the relative coordinate, $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$, and $\mathbf{R}$ is the center-of-mass coordinate, of the two particles, $2\mathbf{R}=\mathbf{r}_1+\mathbf{r}_2$. Since the two-body interaction is a function of $(\mathbf{r}_1-\mathbf{r}_2)$, writing the wave function in terms of $\mathbf{r}$ and $\mathbf{R}$ circumvents the need for expanding the potential in terms of its Slater integrals. In fact, since $\psi(\mathbf{r})$ is a polynomial in $\mathbf{r}$ multiplied by an angular factor (which integrates out) one sees that the calculation of nuclear pairing energies becomes the problem of calculating "moments" of the two-body interaction weighted by appropriate expansion coefficients. Several authors[3] have dealt with the problem of calculating these expansion (or Talmi) coefficients. Generally the procedure for finding them depends on tedious algebra and, moreover, is based on the assumption that the nuclear wave function commutes with the two-body interaction.

In this note we give an operator which allows one to write down explicitly the form of the two-body wave function in terms of $\mathbf{r}$ and $\mathbf{R}$ provided both nucleons are in the same oscillator level. Once this is done one can calculate the Talmi coefficients and, further, can easily treat the case that the two-body interaction has a velocity-dependent part.

THEORY

If we write the oscillator Hamiltonian for a single particle as

$$H_1=(p_1^2/2m)+\tfrac{1}{2}kr_1^2, \tag{1}$$

then a solution corresponding to energy $E=(\hbar^2k/m)^{\frac{1}{2}}\times(2n+l+\frac{3}{2})$ is given by

$$\psi=\chi_{nl}(r_1)Y_l^m(\theta_1,\phi_1), \tag{2}$$

where the normalized form of the radial wave function is

$$\chi_{nl}(r_1)=\left[\frac{2^{l-n+2}(2l+2n+1)!!\alpha^{(2l+3)/2}}{\pi^{\frac{1}{2}}n![(2l+1)!!]^2}\right]^{\frac{1}{2}}\exp(-\alpha r_1^2/2)r_1^l\sum_{k=0}^{n}\frac{(-1)^k2^kn!(2l+1)!!(\alpha r_1^2)^k}{k!(n-k)!(2l+2k+1)!!}, \tag{3}$$

with $\alpha=(mk/\hbar^2)^{\frac{1}{2}}$ and $Y_l^m(\theta_1,\phi_1)$ the usual spherical harmonic. Our notation is such that the lowest state of any l is denoted with $n=0$, namely $(0l)$. Also $(2l+1)!!\equiv1\times3\times5\times\cdots\times(2l+1)$.

Using Eq. (2) one easily writes down the eigenfunction for two particles moving in the same oscillator potential and coupling their spins to a resultant J, with z component M. If one of the particles has quantum numbers n, l

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* Work performed under the auspices of the U. S. Atomic Energy Commission.

† An abstract of this work was originally reported at the 1959 Annual Meeting of the American Physical Society [Bull. Am. Phys. Soc. 4, 49 (1959)].

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[1] See for example E. U. Condon and G. H. Shortley, *Theory of Atomic Spectra* (Cambridge University Press, London, 1951).

[2] I. Talmi, Helv. Phys. Acta **25**, 185 (1952).

[3] E. H. Kronheimer, Phys. Rev. **90**, 1003 (1953); G. E. Tauber and T. Y. Wu, Phys. Rev. **94**, 1307 (1954); J. M. Kennedy, Chalk River (unpublished); W. W. True, Princeton (unpublished); R. Thieberger, Nuclear Phys. **2**, 533 (1956/57); K. W. Ford and E. J. Konopinski, Nuclear Phys. **9**, 218 (1958/59).

and the other $n'l'$, then in j–j coupling the wave function is

$$\psi_J{}^{M'}=\chi_{nl}(r_1)\chi_{n'l'}(r_2)\sum_{mm'}C_{jj'}(JM';mm')\mathcal{Y}_j{}^m(1)\mathcal{Y}_{j'}{}^{m'}(2), \tag{4}$$

where $C_{jj'}(JM';mm')$ is the Clebsch-Gordan coefficient which insures that j and j' couple to J and $\mathcal{Y}_j{}^m$ denotes a space-spin eigenfunction in which the orbital angular momentum l and spin angular momentum $\frac{1}{2}$ are compounded to give j. In the absence of two-body forces, the energy of the state $\psi_J{}^{M'}$ does not depend on J and is given by

$$E=(\hbar^2k/m)^{\frac{1}{2}}(2n+2n'+l+l'+3). \tag{5}$$

Since we wish to write the spatial part of the wave function in terms of $\mathbf{r}$ and $\mathbf{R}$, it is convenient to work in the L–S coupling scheme. In this representation $\psi_J{}^{M'}$ given by Eq. (4) becomes

$$\psi_J{}^{M'}=\chi_{nl}(r_1)\chi_{n'l'}(r_2)\sum_{LS}\gamma_L{}^S\sum_{MM_s}C_{LS}(JM';MM_s)Y_L{}^M\chi_S{}^{M_s}, \tag{6}$$

where $\chi_S{}^{M_s}$ is the spin eigenfunction of the two particles, S taking on the values 0 or 1, $Y_L{}^M$ is the orbital angular momentum eigengunction obtained from combining l and l', namely,

$$Y_L{}^M=\sum_{mm'}C_{ll'}(LM;mm')Y_l{}^m(1)Y_{l'}{}^{m'}(2). \tag{7}$$

Here $L=J$, $J\pm1$, and $\gamma_L{}^S$, which are $(9j)$ symbols,[4] are the j–j to LS transformation coefficients, and have the values[5]

$$\begin{aligned}
\gamma_J{}^0&=\tfrac{1}{2}\left\{1+\frac{(-1)^{j+j'-l-l'}2[J(J+1)-j(j+1)-j'(j'+1)]}{(2l+1)(2l'+1)}\right\}^{\frac{1}{2}},\\
\gamma_J{}^1&=\frac{[(l+\frac{1}{2})+(-1)^{j+j'-l-l'}(l'+\frac{1}{2})]}{[J(J+1)]^{\frac{1}{2}}}\gamma_J{}^0,\\
\gamma_{J+1}{}^1&=(-1)^{j-l+\frac{1}{2}}\left[\frac{(-1)^{j-j'-l-l'}(l+l'-J)(l+l'-J+1)(l'-l+J+1)(l-l'+J+1)}{2(2l+1)(2l'+1)(J+1)(2J+1)}\right]^{\frac{1}{2}},\\
\gamma_{J-1}{}^1&=(-1)^{j'-l'-\frac{1}{2}}\left[\frac{(-1)^{j-j'-l-l'}(l+l'+J+2)(l-l'+J)(l'-l+J)(l+l'+J+1)}{2(2l+1)(2l'+1)J(2J+1)}\right]^{\frac{1}{2}}.
\end{aligned} \tag{8}$$

The first equation holds for all j, j', l, and l'. The same is true of the second except that when $j=l-\frac{1}{2}$ and $j'=l'-\frac{1}{2}$ the equation must be multiplied by minus one. On the other hand, the last two equations, aside from the phase factors both inside and outside the radical sign, hold only for $j=l+\frac{1}{2}$, $j'=l'+\frac{1}{2}$. To obtain the analogous equations when $j=l-\frac{1}{2}$ $(j'=l'-\frac{1}{2})$, one replaces l by $-(l+1)$ [l' by $-(l'+1)$] in each of the four factors in the numerator of the expressions.

The problem now is to express

$$\phi_L{}^M=\chi_{nl}(r_1)\chi_{n'l'}(r_2)Y_L{}^M(1,2)$$

in terms of the relative coordinate

$$\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2 \tag{9}$$

and the center-of-mass coordinate

$$\mathbf{R}=\tfrac{1}{2}(\mathbf{r}_1+\mathbf{r}_2). \tag{10}$$

To do this we first note that if Eqs. (9) and (10) define our new coordinate system, then the canonical momenta conjugate to these are given by

$$\mathbf{p}=\tfrac{1}{2}(\mathbf{p}_1-\mathbf{p}_2), \tag{11}$$

$$\mathbf{P}=\mathbf{p}_1+\mathbf{p}_2. \tag{12}$$

Using Eqs. (9), (10), (11), and (12), we see that the total Hamiltonian of the two particles, $H=H_1+H_2$ is again separable into the sum of two harmonic oscillators. Further we have the restriction that the eigenfunction represents a state whose energy is given by Eq. (5). Thus if (n_1,l_1) refer to the quantum numbers associated with the relative motion and (n_2,l_2) those for the center of mass, it follows that

$$2n+2n'+l+l'=2n_1+2n_2+l_1+l_2. \tag{13}$$

For simplicity we shall abbreviate the combination

$$R_{n_1l_1}(r)\mathcal{R}_{n_2l_2}(R)\sum_{m_1m_2}C_{l_1l_2}(LM;m_1m_2)Y_{l_1}{}^{m_1}(\theta)Y_{l_2}{}^{m_2}(\Theta)=\{U_{n_1l_1}\mathcal{U}_{n_2l_2}\}_{LM}. \tag{14}$$

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[4] See for example A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, 1957).

[5] G. Racah, Physica **16**, 651 (1950); M. H. L. Pryce, Proc. Phys. Soc. (London) **A65**, 773 (1952); Arima, Horie, and Tanabe, Progr. Theoret. Phys. (Kyoto) **11**, 143 (1954).

It has to be borne in mind that in the radial wave function $R_{n_1l_1}(r)$ for the relative motion, the α occurring in Eq. (3) has to be replaced by $\alpha/2$; for $\mathcal{R}_{n_2l_2}(R)$, α has to be replaced by 2α. In the new coordinate system $\phi_L{}^M$ may then be written as

$$\phi_L{}^M=\sum_{n_1l_1n_2l_2} a(n_1l_1;\, n_2l_2)\{U_{n_1l_1}\mathfrak{U}_{n_2l_2}\}_{LM}. \qquad (15)$$

The summation is restricted by Eq. (13).

We now have to determine the expansion coefficients $a(n_1l_1;\, n_2l_2)$. Let us consider two-particle wave functions which arise when both particles are in the same oscillator level (i.e., when both particles have the same energy although not necessarily the same radial and angular quantum numbers). This wave function must be antisymmetric to the exchange of the two particles. From this it follows that for isotopic spin one and spin zero as well as for $T=0$, $S=1$, $\phi_L{}^M$ can contain only even values of l_1 (and hence l_2). In the case $T=1$, $S=1$ or $T=0$, $S=0$, only odd l_1 and l_2 occur. Further, the space reflection $\mathbf{r}_2\rightarrow-\mathbf{r}_2$ multiplies the wave function by $(-1)^{l'}$. Since under this transformation $\mathbf{r}\rightarrow 2\mathbf{R}$ so $\mathbf{R}\rightarrow\mathbf{r}/2$, it follows that

$$a(n_1l_1;\, n_2l_2)=(-1)^{L+l'}a(n_2l_2;\, n_1l_1), \qquad (16)$$

the factor $(-1)^L$ arising from the interchange of l_1 and l_2 in the Clebsch-Gordan coefficient.

An important restriction on the expansion coefficients in Eq. (15) is obtained by observing that $\phi_L{}^M$, an eigenfunction of H_1+H_2, is also an eigenfunction of H_1 alone, and has energy $E/2$. To see the implication of this, let us transform H_1 to relative and center-of-mass coordinates.

$$H_1=\tfrac{1}{2}\left[\frac{P^2}{4m}+kR^2+\frac{p^2}{m}+\tfrac{1}{4}kr^2\right]+\frac{\mathbf{p}\cdot\mathbf{P}}{2m}+\tfrac{1}{2}k\mathbf{r}\cdot\mathbf{R}. \qquad (17)$$

However, expressed in the new coordinate system the wave function is an eigenfunction of the term in brackets and has eigenvalue $E/2$. Hence the sum of the last two terms when operating on the wave function must be zero. This implies

$$2\left(\frac{m}{\hbar^2k}\right)^{\frac{1}{2}}\left(\frac{\mathbf{p}\cdot\mathbf{P}}{2m}+\tfrac{1}{2}k\mathbf{r}\cdot\mathbf{R}\right)\phi_L{}^M=E_+\phi_L{}^M=0, \qquad (18)$$

where the multiplicative factor has been introduced for later convenience. The effect of this operator on a typical term in the wave function is easily calculated by the standard Racah techniques[6] and gives

$$\begin{aligned}E_+\{U_{n_1l_1}\mathfrak{U}_{n_2l_2}\}_{LM}=-\frac{1}{\alpha}\sum_{L_1L_2}\Bigg\{&\left(\frac{\partial}{\partial r}-\frac{l_1}{r}\delta_{L_1,\,l_1+1}+\frac{l_1+1}{r}\delta_{L_1,\,l_1-1}\right)\left(\frac{\partial}{\partial R}-\frac{l_2}{R}\delta_{L_2,\,l_2+1}+\frac{l_2+1}{R}\delta_{L_2,\,l_2-1}\right)-\alpha^2rR\Bigg\}\\ &\times(-1)^{L+L_2-l_1}[(2l_1+1)(2l_2+1)]^{\frac{1}{2}}C_{1l_1}(L_10;\,00)C_{1l_2}(L_20;\,00)\\ &\times W(l_1L_1l_2L_2;\,1L)\sum_{M_1M_2}C_{L_1L_2}(LM;\,M_1M_2)Y_{L_1}{}^{M_1}(\theta)Y_{L_2}{}^{M_2}(\Theta), \qquad (19)\end{aligned}$$

where the W's are the Racah coefficients.[6] By use of the form of the radial wave function, Eq. (3), together with the appropriate modification of α discussed previously, and the simple form of the Clebsch-Gordan coefficient when all the m's are zero,[6] this equation becomes

$$\begin{aligned}E_+\{U_{n_1l_1}\mathfrak{U}_{n_2l_2}\}_{LM}=(-1)^{L+l_1+l_2}\big[&([2n_2(2l_1+2n_1+3)]^{\frac{1}{2}}\{U_{n_1,\,l_1+1}\mathfrak{U}_{n_2-1,\,l_2+1}\}_{LM}\\ &+[2n_1(2l_2+2n_2+3)]^{\frac{1}{2}}\{U_{n_1-1,\,l_1+1}\mathfrak{U}_{n_2,\,l_2+1}\}_{LM})[(l_1+1)(l_2+1)]^{\frac{1}{2}}\\ &\times W(l_1,\,l_1+1,\,l_2,\,l_2+1;\,1,\,L)+(2[n_1(n_2+1)]^{\frac{1}{2}}\{U_{n_1-1,\,l_1+1}\mathfrak{U}_{n_2+1,\,l_2-1}\}_{LM}\\ &+[(2l_1+2n_1+3)(2l_2+2n_2+1)]^{\frac{1}{2}}\{U_{n_1,\,l_1+1}\mathfrak{U}_{n_2,\,l_2-1}\}_{LM})[l_2(l_1+1)]^{\frac{1}{2}}\\ &\times W(l_1,\,l_1+1,\,l_2,\,l_2-1;\,1,\,L)+(2[n_2(n_1+1)]^{\frac{1}{2}}\{U_{n_1+1,\,l_1-1}\mathfrak{U}_{n_2-1,\,l_2+1}\}_{LM}\\ &+[(2l_1+2n_1+1)(2l_2+2n_2+3)]^{\frac{1}{2}}\{U_{n_1,\,l_1-1}\mathfrak{U}_{n_2,\,l_2+1}\}_{LM})[l_1(l_2+1)]^{\frac{1}{2}}\\ &\times W(l_1,\,l_1-1,\,l_2,\,l_2+1;\,1,\,L)+([2(n_1+1)(2l_2+2n_2+1)]^{\frac{1}{2}}\\ &\times\{U_{n_1+1,\,l_1-1}\mathfrak{U}_{n_2,\,l_2-1}\}_{LM}+[2(n_2+1)(2l_1+2n_1+1)]^{\frac{1}{2}}\\ &\qquad\times\{U_{n_1,\,l_1-1}\mathfrak{U}_{n_2+1,\,l_2-1}\}_{LM})[l_1l_2]^{\frac{1}{2}}W(l_1,\,l_1-1,\,l_2,\,l_2-1;\,1,\,L)\big]. \qquad (20)\end{aligned}$$

Although the Racah coefficients involved in this equation have a simple form,[7] we have chosen not to write them out explicitly since many tables of these functions exist.[8]

Thus we see that the operator E_+ leads to an interrelationship between the various coefficients appearing in the expansion of the wave function. However, the wave function is determined uniquely by this operator only under very special circumstances. One may easily see this by taking a specific example. Consider the oscillator shell in which the $(0f)$ and $(1p)$ states are degenerate. In this case there is only one way to construct a state with $L=5$ or 6, namely from the $(0f)^2$

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[6] G. Racah, Phys. Rev. **62**, 438 (1942).

[7] See for example Biedenharn, Blatt, and Rose, Revs. Modern Phys. **24**, 249 (1952).

[8] See for example K. M. Howell, University of Southampton, Research Report US 58-1, June, 1958 (unpublished); Rotenberg, Bivins, Metropolis, and Wooten, *Tables of the 3-j and 6-j Coefficients* (Technology Press, Cambridge, 1960).

configuration, hence E_+ gives these states uniquely (aside from a phase factor). On the other hand the state with $L=4$ can be derived from either the configuration $(0f)^2$ or $(0f,1p)$. Since the E_+ operator arises from considerations which are independent of the angular momenta originally making up the state, it is obvious that alone it cannot differentiate between these two states. One could, of course, look at the operator $L_1^2+L_2^2$, which gives more detailed information about the structure of the state. However, a moment's reflection shows that when this is transformed to relative and center-of-mass coordinates and allowed to operate on a typical term in $\phi_L{}^M$ it can change l_1 to $l_1\pm 2$, 0 and l_2 to $l_2\pm 2$, 0, giving a total of nine terms as compared to four arising from the E_+ operator. However, it is possible, and much simpler, to sort out the ambiguities involved by considering the form of the radial part of the oscillator wave functions. We shall therefore treat the various possible configurations separately, giving additional interrelationships between the expansion coefficients which will be sufficient to determine the wave functions uniquely.

$(0l)^2$ CONFIGURATION

One can supplement the interrelationships between the various a's of Eq. (15) by considering the radial form of the oscillator wave functions, Eq. (3). For the case in which both particles have the same l and no radial nodes, the radial part of the eigenfunction before the transformation of coordinates is proportional to $r_1{}^l r_2{}^l \exp(-\alpha r_1{}^2/2)\exp(-\alpha r_2{}^2/2)$. In the new coordinate system a typical term in the expansion of the wave function must, therefore, have a radial dependence of the form

$$\exp(-\alpha r^2/4)\exp(-\alpha R^2)\sum_{st} b_{st} r^s R^t, \tag{21}$$

where $s+t=2l$. This immediately provides us with some additional restrictions on the expansion coefficients of Eq. (15). For example, if $\phi_L{}^M$ is to represent a state with $L=4$ compounded from the configuration $(0f)^2$, it will contain a term of the form

$$\{aR_{10}(r)\mathcal{R}_{04}(R)+bR_{00}(r)\mathcal{R}_{14}(R)\}\times\sum_{mm'} C_{04}(4M;m_1m_2)Y_0{}^m(\theta)Y_4{}^{m'}(\Theta). \tag{22}$$

The braces contain terms in R^6, r^2R^4, and R^4. Equation (21) tells us that the coefficient of R^4 must be zero. This determines the ratio a/b. We can, of course, have more complicated cases in which the brace contains more than two terms. However, even in these cases Eq. (21) is sufficient to determine the relationship between the coefficients. These relationships are given in Table I and together with the E_+ operator and normalization provide a complete description, aside from a phase factor, of the state in question.

For many two-body interactions the phases of the various components of the wave function, Eq. (6), are unimportant for diagonal matrix elements (the tensor interaction of course provides an exception to this rule). However, the phases are of consequence when off-diagonal matrix elements of the two-body interaction are calculated. Although the operators we have constructed do not give the phases involved, they are easily obtained as follows.

Let us consider singlet spin eigenfunctions which are multiplied by wave functions of isotopic spin one. In this case $\phi_L{}^M$, before the transformation of coordinates, is given by

$$\phi_L{}^M=\left[\frac{2^{l+2}\alpha^{(2l+3)/2}}{\pi^{\frac{1}{2}}(2l+1)!!}\right]\exp[-\alpha(r_1{}^2+r_2{}^2)/2]r_1{}^l r_2{}^l\sum_{mm'} C_{ll}(LM;mm')Y_l{}^m(\theta_1)Y_l{}^{m'}(\theta_2). \tag{23}$$

The limit $\mathbf{r}_1\rightarrow\mathbf{r}_2$ implies that $\mathbf{r}\rightarrow 0$, $\mathbf{R}\rightarrow\mathbf{r}_2=\mathbf{r}_1$, $\Theta\rightarrow\theta_2=\theta_1$, $\Phi\rightarrow\phi_2=\phi_1$. If we use the fact that two spherical harmonics of the same coordinates can be written as[9]

$$Y_l{}^mY_l{}^{m'}=\sum_{L_1M_1}\frac{2l+1}{[4\pi(2L_1+1)]^{\frac{1}{2}}}C_{ll}(L_10;00)C_{ll}(L_1M_1;mm')Y_{L_1}{}^{M_1}, \tag{24}$$

we find

$$\lim_{\mathbf{r}_1\rightarrow\mathbf{r}_2}\phi_L{}^M\rightarrow\left[\frac{2^{l+2}\alpha^{(2l+3)/2}}{\pi^{\frac{1}{2}}(2l+1)!!}\right]\exp(-\alpha R^2)R^{2l}\frac{2l+1}{[4\pi(2L+1)]^{\frac{1}{2}}}C_{ll}(L0;00)Y_L{}^M(\Theta). \tag{25}$$

As a function of r and R, this limit is the term R^{2l} in the expression

$$a\left(0,0;\frac{L-2l}{2},L\right)R_{00}(0)\mathcal{R}_{(L-2l)/2,\,L}Y_0{}^0(0)Y_L{}^M(\Theta).$$

This not only gives the phase of the wave function, $(-1)^{l+L/2}$, but also provides an algebraic check since it gives the numerical value of one of the coefficients in the wave function.

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[9] See for example J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley and Sons, New York, 1952).

TABLE I. The expansion coefficients of the wave function, Eq. (15), are limited by the radial form of the oscillator wave functions. These restrictions are listed for several given oscillator levels.

Term in expansion	Configuration	Restrictions arising from form of oscillator wave functions
$aR_{1l_1}\mathcal{R}_{0l_2}+bR_{0l_1}\mathcal{R}_{1l_2}$	$(0l)^2$	$b=-\left[\frac{2l_1+3}{2l_2+3}\right]^{\frac{1}{2}}a$
$aR_{2l_1}\mathcal{R}_{0l_2}+bR_{1l_1}\mathcal{R}_{1l_2}$ $+cR_{0l_1}\mathcal{R}_{2l_2}$	$(0l)^2$	$b=-\left[\frac{2(2l_1+5)}{2l_2+3}\right]^{\frac{1}{2}}a;\quad c=\left[\frac{(2l_1+3)(2l_1+5)}{(2l_2+3)(2l_2+5)}\right]^{\frac{1}{2}}a$
	$\{0l,\ 1(l-2)\}$	$[(2l_1+3)(2l_1+5)]^{\frac{1}{2}}a+[2(2l_1+3)(2l_2+3)]^{\frac{1}{2}}b+[(2l_2+3)(2l_2+5)]^{\frac{1}{2}}c=0$
$aR_{3l_1}\mathcal{R}_{0l_2}+bR_{2l_1}\mathcal{R}_{1l_2}$ $+cR_{1l_1}\mathcal{R}_{2l_2}+dR_{0l_1}\mathcal{R}_{3l_2}$	$(0l)^2$	$b=-\left[\frac{3(2l_1+7)}{2l_2+3}\right]^{\frac{1}{2}}a;\ c=\left[\frac{3(2l_1+5)(2l_1+7)}{(2l_2+3)(2l_2+5)}\right]^{\frac{1}{2}}a;\ d=-\left[\frac{(2l_1+7)!!(2l_2+1)!!}{(2l_1+1)!!(2l_2+7)!!}\right]^{\frac{1}{2}}a$
	$\{0l,\ 1(l-2)\}$	$[3(2l_1+5)(2l_1+7)]^{\frac{1}{2}}a+2[(2l_1+5)(2l_2+3)]^{\frac{1}{2}}b+[(2l_2+3)(2l_2+5)]^{\frac{1}{2}}c=0$ $\left[\frac{(2l_1+7)!!}{3(2l_1+1)!!}\right]^{\frac{1}{2}}a+\left[\frac{(2l_1+5)!!(2l_2+3)!!}{(2l_1+1)!!(2l_2+1)!!}\right]^{\frac{1}{2}}b$ $+\left[\frac{(2l_1+3)!!(2l_2+5)!!}{(2l_1+1)!!(2l_2+1)!!}\right]^{\frac{1}{2}}c+\left[\frac{(2l_2+7)!!}{3(2l_2+1)!!}\right]^{\frac{1}{2}}d=0\,(\mathrm{I})$
	$\{0l,\ 2(l-4)\}$ or $\{1(l-2)\}^2$	$I=0$
$aR_{4l_1}\mathcal{R}_{0l_2}+bR_{3l_1}\mathcal{R}_{1l_2}$ $+cR_{2l_1}\mathcal{R}_{2l_2}+dR_{1l_1}\mathcal{R}_{3l_2}$ $+eR_{0l_1}\mathcal{R}_{4l_2}$	$(0l)^2$	$b=-2\left[\frac{2l_1+9}{2l_2+3}\right]^{\frac{1}{2}}a;\quad c=\left[\frac{6(2l_1+7)(2l_1+9)}{(2l_2+3)(2l_2+5)}\right]^{\frac{1}{2}}a;$ $d=-2\left[\frac{(2l_1+9)!!(2l_2+1)!!}{(2l_1+3)!!(2l_2+7)!!}\right]^{\frac{1}{2}}a;\quad e=\left[\frac{(2l_1+9)!!(2l_2+1)!!}{(2l_1+1)!!(2l_2+9)!!}\right]^{\frac{1}{2}}a$
	$\{0l,\ 1(l-2)\}$	$\mathrm{II}=[(2l_1+3)(2l_1+5)]^{\frac{1}{2}}c+[6(2l_1+3)(2l_2+7)]^{\frac{1}{2}}d+[6(2l_2+7)(2l_2+9)]^{\frac{1}{2}}e=0$ $\mathrm{III}=[3(2l_1+5)(2l_1+7)]^{\frac{1}{2}}b+2[2(2l_1+5)(2l_2+5)]^{\frac{1}{2}}c+[3(2l_2+5)(2l_2+7)]^{\frac{1}{2}}d=0$ $\mathrm{IV}=[6(2l_1+9)(2l_1+7)]^{\frac{1}{2}}a+[6(2l_1+7)(2l_2+3)]^{\frac{1}{2}}b+[(2l_2+3)(2l_2+5)]^{\frac{1}{2}}c=0$
	$\{0l;\ 2(l-4)\}$ or $\{1(l-2)\}^2$	$[2(2l_2+5)]^{\frac{1}{2}}\mathrm{II}+[2l_1+3]^{\frac{1}{2}}\mathrm{III}=0$ $[(2l_2+3)]^{\frac{1}{2}}\mathrm{III}+[2(2l_1+5)]^{\frac{1}{2}}\mathrm{IV}=0$
	$\{1(l-2),\ 2(l-4)\}$	$[(2l_2+3)(2l_2+5)]^{\frac{1}{2}}\mathrm{II}+[2(2l_1+3)(2l_2+3)]^{\frac{1}{2}}\mathrm{III}+[(2l_1+3)(2l_1+5)]^{\frac{1}{2}}\mathrm{IV}=0$
$aR_{5l_1}\mathcal{R}_{0l_2}+bR_{4l_1}\mathcal{R}_{1l_2}$ $+cR_{3l_1}\mathcal{R}_{2l_2}+dR_{2l_1}\mathcal{R}_{3l_2}$ $+eR_{1l_1}\mathcal{R}_{4l_2}+fR_{0l_1}\mathcal{R}_{5l_2}$	$(0l)^2$	$b=-\left[\frac{5(2l_1+11)}{2l_2+3}\right]^{\frac{1}{2}}a;\quad c=\left[\frac{10(2l_1+9)(2l_1+11)}{(2l_2+3)(2l_2+5)}\right]^{\frac{1}{2}}a;$ $d=-\left[\frac{10(2l_1+11)!!(2l_2+1)!!}{(2l_1+5)!!(2l_2+7)!!}\right]^{\frac{1}{2}}a;\quad e=\left[\frac{5(2l_1+11)!!(2l_2+1)!!}{(2l_1+3)!!(2l_2+9)!!}\right]^{\frac{1}{2}}a;$ $f=-\left[\frac{(2l_1+11)!!(2l_2+1)!!}{(2l_1+1)!!(2l_2+11)!!}\right]^{\frac{1}{2}}a$
	$\{0l,\ 1(l-2)\}$	$\mathrm{V}=[10(2l_1+9)(2l_1+11)]^{\frac{1}{2}}a+2[2(2l_1+9)(2l_2+3)]^{\frac{1}{2}}b+[(2l_2+3)(2l_2+5)]^{\frac{1}{2}}c=0$ $\mathrm{VI}=[2(2l_1+7)(2l_1+9)]^{\frac{1}{2}}b+2[(2l_1+7)(2l_2+5)]^{\frac{1}{2}}c+[(2l_2+5)(2l_2+7)]^{\frac{1}{2}}d=0$ $\mathrm{VII}=[(2l_1+5)(2l_1+7)]^{\frac{1}{2}}c+2[(2l_1+5)(2l_2+7)]^{\frac{1}{2}}d+[2(2l_2+7)(2l_2+9)]^{\frac{1}{2}}e=0$ $\mathrm{VIII}=[(2l_1+3)(2l_1+5)]^{\frac{1}{2}}d+2[2(2l_1+3)(2l_2+9)]^{\frac{1}{2}}e+[10(2l_2+9)(2l_2+11)]^{\frac{1}{2}}f=0$
	$\{0l,\ 2(l-4)\}$ or $\{1(l-2)\}^2$	$[(2l_1+7)]^{\frac{1}{2}}\mathrm{V}+[(2l_2+3)]^{\frac{1}{2}}\mathrm{VI}=0$ $[(2l_1+5)]^{\frac{1}{2}}\mathrm{VI}+[(2l_2+5)]^{\frac{1}{2}}\mathrm{VII}=0$ $[(2l_1+3)]^{\frac{1}{2}}\mathrm{VII}+[(2l_2+7)]^{\frac{1}{2}}\mathrm{VIII}=0$
	$\{1(l-2),\ 2(l-4)\}$	$[(2l_1+5)(2l_1+7)]^{\frac{1}{2}}\mathrm{V}+2[(2l_1+5)(2l_2+3)]^{\frac{1}{2}}\mathrm{VI}+[(2l_2+3)(2l_2+5)]^{\frac{1}{2}}\mathrm{VII}=0$ $[(2l_1+3)(2l_1+5)]^{\frac{1}{2}}\mathrm{VI}+2[(2l_1+3)(2l_2+5)]^{\frac{1}{2}}\mathrm{VII}+[(2l_2+5)(2l_2+7)]^{\frac{1}{2}}\mathrm{VIII}=0$
	$\{2(l-4)\}^2$	$\left[\frac{(2l_1+7)!!}{(2l_1+1)!!}\right]^{\frac{1}{2}}\mathrm{V}+3\left[\frac{(2l_1+5)!!(2l_2+3)}{(2l_1+1)!!}\right]^{\frac{1}{2}}\mathrm{VI}$ $+3\left[\frac{(2l_1+3)(2l_2+5)!!}{(2l_2+1)!!}\right]^{\frac{1}{2}}\mathrm{VII}+\left[\frac{(2l_2+7)!!}{(2l_2+1)!!}\right]^{\frac{1}{2}}\mathrm{VIII}=0$

Only odd values of L occur in the $\phi_L{}^M$ multiplying the triplet spin eigenfunction. One cannot immediately go to the limit $r_1=r_2$, since the wave function always contains a term $\sim rY_1{}^m(\theta)$. In this case it is convenient to expand $r_1{}^l Y_l{}^m(\theta_1)$ in a Taylor series about the point r_2, θ_2, ϕ_2 so that

$$
\begin{aligned}
r_1{}^l Y_l{}^m(\theta_1) &\sim r_2{}^l Y_l{}^m(\theta_2)+(\mathbf{r}_1-\mathbf{r}_2)\cdot(\nabla r^l Y_l{}^m)_{\mathbf{r}_2}+\tfrac{1}{2}\sum_{st}(r_1-r_2)_s(r_1-r_2)_t(\nabla_s\nabla_t r^l Y_l{}^m)_{\mathbf{r}_2} \\
&= r_2{}^l Y_l{}^m(\theta_2)-rr_2{}^{l-1}(2l+1)\left[\frac{4\pi l}{3(2l-1)}\right]^{\frac{1}{2}}\sum_{m_1M}(-1)^{m_1}C_{l1}(l-1,M;m-m_1)Y_1{}^{m_1}(\theta)Y_{l-1}{}^M(\theta_2) \\
&\quad +r^2r_2{}^{l-2}\left[\frac{4\pi l(l-1)(2l-1)(2l+1)}{30}\right]^{\frac{1}{2}}\sum_{m_1m_2}C_{2,\,l-2}(lm;m_1m_2)Y_2{}^{m_1}(\theta)Y_{l-2}{}^{m_2}(\theta_2), \qquad (26)
\end{aligned}
$$

where we have made use of the fact that the m_1th component of $\mathbf{r}_1-\mathbf{r}_2$ may be written as a function of the relative coordinates only and is proportional to $rY_1{}^{m_1}$. Although they are unnecessary at present, we have also retained terms of order r^2 since we shall need them when we consider two particles in states with different angular momentum. The first term in Eq. (26), of course, gives no contribution when substituted into Eq. (23) since it is impossible to combine $Y_l{}^m(\theta_2)Y_l{}^{m'}(\theta_2)$ to total angular momentum L, when L is odd. The second term, however, does not vanish so that

$$
\begin{aligned}
\lim_{\mathbf{r}_1\to\mathbf{r}_2}\phi_L{}^M &\to (2l+1)\left[\frac{l(2l+1)(2l-1)}{3}\right]^{\frac{1}{2}}C_{l-1,\,l}(L0;00)W(l,l-1,L,L;1,l) \\
&\quad \times rR^{2l-1}\sum_{m_1m_2}C_{1L}(LM;m_1m_2)Y_1{}^{m_1}(\theta)Y_L{}^{m_2}(\Theta), \qquad (27)
\end{aligned}
$$

yielding a phase $(-1)^{\frac{1}{2}(2l+L+1)}$.

$(1l)^2$ CONFIGURATION

When both wave functions making up $\phi_L{}^M$ have the same l and one radial node it follows that the polynomial, Eq. (21), occurring in a typical term must have

$$2l\leq s+t\leq 2l+4.$$

For terms similar to Eq. (22), this imposes certain restrictions on the expansion coefficients. These are listed in Table I under the heading $(1,l-2)^2$. The reason for the change in notation from the text is that we have written in this table all the possible configurations arising from a particular oscillator shell. Since the ratios of the coefficients do not explicitly depend on l, the same formulas hold independently of the angular momenta of the original states making up the wave function.

Equations (25) and (27), which determine the phase of the wave function, are merely multiplied by

$$\frac{2l+3}{2}\left(1-\frac{2\alpha R^2}{2l+3}\right)^2,$$

which gives both phase and numerical value of one coefficient.

There is an additional simple relationship between the expansion coefficients for the $(1l)^2$ configuration which may be seen as follows. One can construct the wave function $\phi_L{}^M$ for $(1l)^2$ from a knowledge of the $\phi_L{}^M$ arising from $(0l)^2$ by merely multiplying the latter quantity by

$$\frac{2l+3}{2}\left(1-\frac{2\alpha r_1{}^2}{2l+3}\right)\left(1-\frac{2\alpha r_2{}^2}{2l+3}\right).$$

On transforming to relative and center-of-mass coordinates, we find

$$
\begin{aligned}
\phi_L{}^M\{(1l)^2\} &= \frac{2l+3}{2}\biggl\{1-\frac{2\alpha}{2l+3}(2R^2+\tfrac{1}{2}r^2)+\frac{4\alpha^2}{(2l+3)^2} \\
&\quad \times[(R^2+\tfrac{1}{4}r^2)^2+(\mathbf{r}\cdot\mathbf{R})^2]\biggr\}\phi_L{}^M\{(0l)^2\}. \qquad (28)
\end{aligned}
$$

The $(\mathbf{r}\cdot\mathbf{R})^2$ term is the only one which operates on the angular part of $\phi_L{}^M\{(0l)^2\}$ and this leads to the rule that if any term in $\phi_L{}^M\{(1l)^2\}$ has an angular dependence that conservation of energy forbids in the wave function $\phi_L{}^M\{(0l)^2\}$, then that term must be multiplied by a polynomial, Eq. (21), of degree

$$s+t=2l+4.$$

For example, the $(0d)^2$ configuration coupling to spin $L=4$ has a term

$$R_{00}(r)\mathcal{R}_{04}(R)Y_0{}^0Y_4{}^M,$$

whereas the $(1d)^2$ configuration coupling to the same spin contains a term

$$[aR_{12}(r)\mathcal{R}_{04}(R)+bR_{02}(r)\mathcal{R}_{14}(R)]\times\sum_{mm'}C_{24}(4M;mm')Y_2{}^mY_4{}^{m'},$$

The latter term arises from $(\mathbf{r}\cdot\mathbf{R})^2$ operating on the original wave function and hence the interrelationship between a and b must be the same as for a state with no radial nodes.

Finally the state $\phi_L{}^M\{(1l)^2\}$ must be orthogonal to the state $\phi_L{}^M\{(0,l+2)^2\}$. This requirement provides either an additional relationship between the expansion coefficients or can serve as an algebraic check.

$(2l)^2$ CONFIGURATION

Again in this case the fact that the polynomial, Eq. (21), multiplying a typical term in the wave function is limited to be of degree

$$2l\leq s+t\leq 2l+8,$$

provides certain interrelationships between the expansion coefficients which are given in Table I.

The "phase equations," Eqs. (25) and (27), are merely multiplied by

$$\frac{(2l+3)(2l+5)}{8}\left(1-\frac{4\alpha R^2}{2l+3}+\frac{4\alpha^2R^4}{(2l+3)(2l+5)}\right)^2.$$

The analog of Eq. (28) leads to the rule that any term in $\phi_L{}^M\{(2l)^2\}$ that has an angular dependence that cannot by conservation of energy occur in the wave function $\phi_L{}^M\{(1l)^2\}$ must arise from the factor $(\mathbf{r}\cdot\mathbf{R})^4\phi_L{}^M\{(0l)^2\}$ and hence the function of r and R multiplying it must obey the same requirements as if a nodeless wave function were being constructed. For example in $(2d)^2$ coupling to $L=4$, the coefficients a and b in the term

$$[aR_{14}(r)\mathcal{R}_{06}(R)+bR_{04}(r)\mathcal{R}_{16}(R)]\times\sum_{mm'}C_{46}(4M;mm')Y_4{}^mY_6{}^{m'}$$

must satisfy same conditions as for the nodeless wave function.

$\{0l,1(l-2)\}$ CONFIGURATION

So far we have dealt with the cases in which both particles are in states with the same orbital angular momentum. We now turn our attention to configurations in which the particles have different l's but still lie in the same oscillator level.

Again the fact that the coefficient of any $Y_l{}^mY_{l'}{}^{m'}$ in the transformed wave function must be a polynomial of degree not less than $2l-2$ imposes certain restrictions on the coefficients, which are given in Table I.

The phase of the wave function is algebraically somewhat more complicated to find in this case. This is readily seen by noting that it is now possible to construct a symmetric eigenfunction corresponding to an odd value of L (a situation which cannot arise in any of the previously considered configurations). As a function of relative and center-of-mass variables, the symmetric eigenfunction, Eq. (15), contains only even values of l_1 and l_2. When L is even it is always possible to have a term in which $l_1=0$, $l_2=L$. However, for odd L this is not possible and l_1 must be at least two. Thus to find the phase of the wave function for symmetric eigenfunctions with odd L, we must retain terms of order r^2 in Eq. (26). Since this is the case, it is more convenient to consider the limiting process not for $\phi_L{}^M$ but for

$$\varphi_L{}^M=\phi_L{}^M/\exp[-\alpha(r_1{}^2+r_2{}^2)/2]=\phi_L{}^M/\exp(-\alpha r^2/4)\exp(-\alpha R^2).$$

Many of the "phase equations" are only trivially altered when we study configurations other than $\{0l,1(l-2)\}$. Thus we shall consider the more general configuration $\{nl,n'l'\}$ and then specialize. In this case, $\varphi_L{}^M$ before the transformation of coordinates may be written as

$$\varphi_L{}^M=2^{-\frac{1}{2}}\sum_{mm'}C_{ll'}(LM;mm')\{f_{nl}(r_1)g_{n'l'}(r_2)r_1{}^lr_2{}^{l'}Y_l{}^m(1)Y_{l'}{}^{m'}(2)\pm g_{n'l'}(r_1)f_{nl}(r_2)r_1{}^{l'}r_2{}^lY_{l'}{}^{m'}(1)Y_l{}^m(2)\},\tag{29}$$

where f_{nl} and $g_{n'l'}$ may be obtained immediately from Eq. (3) and the + and − signs go with symmetric and antisymmetric wave functions, respectively.

Let us first consider the symmetric wave function. For L even, we may proceed directly to the limit as before and obtain for the $\{0l,1(l-2)\}$ configuration

$$\lim_{\mathbf{r}_1\to\mathbf{r}_2}\varphi_L{}^M\to\frac{2^{l+1}\alpha^{(2l+1)/2}}{\pi^{\frac{1}{2}}(2l-3)!!}\left[\frac{2l-3}{4\pi(2L+1)}\right]^{\frac{1}{2}}C_{l,\,l-2}(L0;00)R^{2l-2}\left(1-\frac{2\alpha R^2}{2l-1}\right)Y_L{}^M(\Theta)\tag{30}$$

which gives the phase $(-1)^{\frac{1}{2}(2l+L-2)}$.

To find the phase of the symmetric wave function with odd L it is convenient to expand all functions of $\mathbf{r}_1$ involved in Eq. (29) about the point $\mathbf{r}_2$. When this is done one sees that in general there will be five terms which can give rise to an r^2 dependence of the transformed wave function. Thus

$$\begin{aligned}\varphi_L{}^M\to 2^{-\frac{1}{2}}\sum_{mm'}C_{ll'}(LM;mm')\Big[&f_{nl}(r_2)g_{n'l'}(r_2)\Big\{\tfrac{1}{2}\sum_{st}r_sr_t(\nabla_s\nabla_tr_1{}^lY_l{}^m)_{\mathbf{r}_2}r_2{}^{l'}Y_{l'}{}^{m'}(\theta_2)+\tfrac{1}{2}\sum_{st}r_sr_t(\nabla_s\nabla_tr_1{}^{l'}Y_{l'}{}^{m'})_{\mathbf{r}_2}\\&\times r_2{}^lY_l{}^m(\theta_2)\Big\}+g_{n'l'}(r_2)\mathbf{r}\cdot(\boldsymbol{\nabla}f_{nl})_{\mathbf{r}_2}\mathbf{r}\cdot(\boldsymbol{\nabla}r_1{}^lY_l{}^m)_{\mathbf{r}_2}r_2{}^{l'}Y_{l'}{}^{m'}(\theta_2)+f_{nl}(r_2)\mathbf{r}\cdot(\boldsymbol{\nabla}g_{n'l'})_{\mathbf{r}_2}\mathbf{r}\cdot(\boldsymbol{\nabla}r_1{}^{l'}Y_{l'}{}^{m'})_{\mathbf{r}_2}r_2{}^lY_l{}^m(\theta_2)\\&+\tfrac{1}{2}\sum_{st}r_sr_t(\nabla_s\nabla_tf_{nl})_{\mathbf{r}_2}g_{n'l'}(r_2)r_2{}^{l+l'}Y_l{}^m(\theta_2)Y_{l'}{}^{m'}(\theta_2)+\tfrac{1}{2}\sum_{st}r_sr_t(\nabla_s\nabla_tg_{n'l'})_{\mathbf{r}_2}f_{nl}(r_2)r_2{}^{l+l'}Y_l{}^m(\theta_2)Y_{l'}{}^{m'}(\theta_2)\Big].\end{aligned}\tag{31}$$

The first term arises from the expansion of $r_1{}^l Y_l{}^m$ and $r_1{}^l Y_{l'}{}^{m'}$ about the point r_2 and is easily evaluated to give

$$f_{nl}(R) g_{n'l'}(R) \frac{r^2 R^{l+l'-2}}{2} \left[\frac{(2l+1)(2l'+1)}{15}\right]^{\frac{1}{2}} \{\sum_{L_2} [l(l-1)(2l+1)(2l-1)(2l-3)]^{\frac{1}{2}} C_{l-2,\, l'}(L_2 0;00)$$

$$\times W(l-2, l, L_2, L; 2, l') - \sum_{L_2} [l'(l'-1)(2l'+1)(2l'-1)(2l'-3)]^{\frac{1}{2}} C_{l'-2,\, l}(L_2 0;00)$$

$$\times W(l'-2, l', L_2, L; 2, l)\} \sum_{m_1 m_2} C_{2L_2}(LM; m_1 m_2) Y_2{}^{m_1}(\theta) Y_{L_2}{}^{m_2}(\Theta). \tag{32}$$

The second and third terms are due to the expansion of f_{nl} and $g_{n'l'}$ about $\mathbf{r}_2$. They are most simply evaluated by noting that

$$\begin{aligned} \mathbf{r}\cdot(\nabla f_{nl})_{\mathbf{r}_2} &= F_{nl}(r_2)\mathbf{r}\cdot\mathbf{r}_2, \\ \mathbf{r}\cdot(\nabla g_{n'l'})_{\mathbf{r}_2} &= G_{n'l'}(r_2)\mathbf{r}\cdot\mathbf{r}_2. \end{aligned} \tag{33}$$

Using this fact, one can show that the first of these two terms gives

$$-F_{nl}(R) g_{n'l'}(R) r^2 R^{l+l'}(2l+1)\left[\frac{l(2l-1)(2l'+1)(2L+1)}{3}\right]^{\frac{1}{2}} C_{l-1,\, l'}(L0;00)$$

$$\times W(l, l-1, L, L; 1, l') \sum_{L_2 m_1 m_2} C_{1L}(L_2 0;00) W(LL12;1L_2) C_{2L_2}(LM; m_1 m_2) Y_2{}^{m_1}(\theta) Y_{L_2}{}^{m_2}(\Theta), \tag{34}$$

and the second becomes

$$G_{n'l'}(R) f_{nl}(R) r^2 R^{l+l'}(2l'+1)\left[\frac{l'(2l'-1)(2l+1)(2L+1)}{3}\right]^{\frac{1}{2}} C_{l'-1,\, l}(L0;00)$$

$$\times W(l', l'-1, L, L; 1, l) \sum_{L_2 m_1 m_2} C_{1L}(L_2 0;00) W(LL12;1L_2) C_{2L_2}(LM; m_1 m_2) Y_2{}^{m_1}(\theta) Y_{L_2}{}^{m_2}(\Theta). \tag{35}$$

The fourth and fifth terms in Eq. (31) give no contribution. This is easily seen as follows. The product $Y_l{}^m Y_{l'}{}^{m'}$ gives, according to Eq. (24), a sum of spherical harmonics—each term in the sum having L_1 even. However, the summation over m and m' implies that $L_1 = L$ and hence the terms vanish for odd L.

Thus the sum of Eqs. (32), (34) and (35) gives the dependence to order r^2 of the symmetric wave function when L is odd and holds quite generally for arbitrary n, l, n' and l'. For the configuration $\{0l, 1(l-2)\}$ one merely sets $l' = l-2$ and from Eq. (3) obtains

$$\begin{aligned} f_{nl} &= \left[\frac{2^{l+2}\alpha^{(2l+3)/2}}{\pi^{\frac{1}{2}}(2l+1)!!}\right]^{\frac{1}{2}}, \\ g_{n'l'} &= \left[\frac{2^{l-1}(2l-1)\alpha^{(2l-1)/2}}{\pi^{\frac{1}{2}}(2l-3)!!}\right]^{\frac{1}{2}}\left(1-\frac{2\alpha R^2}{2l-1}\right), \\ F_{nl} &= 0, \\ G_{n'l'} &= \frac{-4\alpha}{2l-1}\left[\frac{2^{l-1}(2l-1)\alpha^{(2l-1)/2}}{\pi^{\frac{1}{2}}(2l-3)!!}\right]^{\frac{1}{2}}. \end{aligned} \tag{36}$$

For the antisymmetric states the minus sign applies in Eq. (29) and the analog of Eq. (31), which in this case gives the dependence of the wave function to order r, is

$$\varphi_L{}^M \rightarrow 2^{-\frac{1}{2}} \sum_{mm'} C_{ll'}(LM;mm')[f_{nl}(r_2) g_{n'l'}(r_2)\{\mathbf{r}\cdot(\boldsymbol{\nabla} r_1{}^l Y_l{}^m)_{\mathbf{r}_2} r_2{}^{l'} Y_{l'}{}^{m'}(\theta_2) - \mathbf{r}\cdot(\boldsymbol{\nabla} r_1{}^{l'} Y_{l'}{}^{m'})_{\mathbf{r}_2} r_2{}^l Y_l{}^m(\theta_2)\}$$

$$+\{g_{n'l'}\mathbf{r}\cdot(\boldsymbol{\nabla} f_{nl})_{\mathbf{r}_2} - f_{nl}\mathbf{r}\cdot(\boldsymbol{\nabla} g_{n'l'})_{\mathbf{r}_2}\} r_2{}^{l+l'} Y_l{}^m(\theta_2) Y_{l'}{}^{m'}(\theta_2). \tag{37}$$

Again the first term arises from the expansion of $r_1{}^l Y_l{}^m$ and $r_1{}^{l'} Y_{l'}{}^{m'}$ about r_2, and its value is given by

$$f_{nl}(R) g_{n'l'}(R)\left[\frac{(2l+1)(2l'+1)}{6}\right]^{\frac{1}{2}} r R^{l+l'-1} \sum_{m m_1 L_1} C_{1L_1}(LM; m m_1) Y_1{}^m(\theta) Y_{L_1}{}^{m_1}(\Theta)\{[l(2l+1)(2l-1)]^{\frac{1}{2}}$$

$$\times C_{l',\, l-1}(L_1 0;00) W(l, l-1, L, L_1; 1, l') - (-1)^L [l'(2l'+1)(2l'-1) C_{ll'-1}(L_1 0;00) W(l', l'-1, L, L_1; 1, l\}), \tag{38}$$

whereas the second term becomes

$$-\left[\frac{(2l+1)(2l'+1)}{6(2L+1)}\right]^{\frac{1}{2}}\{g_{n'l'}(R)F_{nl}(R)-f_{nl}(R)G_{n'l'}(R)\}$$
$$\times C_{ll'}(L0;00)rR^{l+l'+1}\sum_{mm_1L_1}C_{1L}(L_10;00)C_{1L_1}(LM;mm_1)Y_1{}^{m}(\theta)Y_{L_1}{}^{m_1}(\Theta). \quad (39)$$

For the $\{0l, 1(l-2)\}$ configuration the requisite values of f and g are given by Eqs. (36). Substituting these into Eqs. (38) and (39), and using the fact that $l'=l-2$, gives the phase of the wave function and also the numerical value of some of the coefficients entering into the expansion.

$\{0l, 2(l-4)\}$ CONFIGURATION

The restrictions on the expansion coefficients [imposed by virtue of the degree of the polynomial, Eq. (21), multiplying any angular factor] are again listed in Table I.

The phase of the wave function is obtained in a straightforward manner from the equations derived in the previous section. For symmetric states with even L, the analog of Eq. (30) is

$$\lim_{r_1\to r_2}\varphi_L{}^M\to\frac{2^{l-1}\alpha^{(2l-1)/2}}{\pi^{\frac{1}{2}}(2l-7)!!}\left[\frac{(2l-7)}{4\pi(2l-1)(2L+1)}\right]^{\frac{1}{2}}C_{l,\,l-4}(L0;00)\left(1-\frac{4\alpha R^2}{2l-5}+\frac{4\alpha^2R^4}{(2l-3)(2l-5)}\right)R^{2l-4}Y_L{}^M(\Theta). \quad (40)$$

The signs of the symmetric wave functions with odd L are obtained from Eqs. (32), (34), and (35), whereas the phases of the antisymmetric states are given by (38), and (39). In these equations l' is replaced by $l-4$, f and F are given by Eqs. (36), and

$$g_{n'l'}=\left[\frac{2^{l-5}(2l-3)(2l-5)\alpha^{(2l-5)/2}}{\pi^{\frac{1}{2}}(2l-7)!!}\right]^{\frac{1}{2}}\left(1-\frac{4\alpha R^2}{2l-5}+\frac{4\alpha^2R^4}{(2l-3)(2l-5)}\right),$$

$$G_{n'l'}=\frac{-8\alpha}{2l-5}\left[\frac{2^{l-5}(2l-3)(2l-5)\alpha^{(2l-5)/2}}{\pi^{\frac{1}{2}}(2l-7)!!}\right]^{\frac{1}{2}}\left(1-\frac{2\alpha R^2}{2l-3}\right).$$

$\{1l, 2(l-2)\}$ CONFIGURATION

Table I lists the restrictions on the coefficients imposed by the degree of the polynomial, Eq. (21). For reasons discussed previously, in the table the relationships are listed for the configuration $\{1(l-2), 2(l-4)\}$.

The phase of the wave functions is determined easily from the previous equations. For symmetric wave functions with even L,

$$\lim_{r_1\to r_2}\varphi_L{}^M\to\frac{2^{l-1}\alpha^{(2l+1)/2}}{\pi^{\frac{1}{2}}(2l-3)!!}\left[\frac{2(2l+1)(2l+3)(2l-3)}{4\pi(2L+1)}\right]^{\frac{1}{2}}C_{l,\,l-2}(L0;00)$$
$$\times R^{2l-2}\left(1-\frac{2\alpha R^2}{2l+3}\right)\left(1-\frac{4\alpha R^2}{2l-1}+\frac{4\alpha^2R^4}{(2l-1)(2l+1)}\right)Y_L{}^M(\Theta),$$

with a phase $(-1)^{\frac{1}{2}(2l+L-2)}$.

For the phases of the remaining wave functions, Eqs. (32), (34), (35), (38), and (39) are applicable with $l'=l-2$, and

$$f_{nl}=\left[\frac{2^{l+1}(2l+3)\alpha^{(2l+3)/2}}{\pi^{\frac{1}{2}}(2l+1)!!}\right]^{\frac{1}{2}}\left(1-\frac{2\alpha R^2}{2l+3}\right),$$

$$g_{n'l'}=\left[\frac{2^{l-3}(2l-1)(2l+1)\alpha^{(2l-1)/2}}{\pi^{\frac{1}{2}}(2l-3)!!}\right]^{\frac{1}{2}}\left(1-\frac{4\alpha R^2}{2l-1}+\frac{4\alpha^2R^4}{(2l-1)(2l+1)}\right),$$

$$F_{nl}=\frac{-4\alpha}{2l+3}\left[\frac{2^{l+1}(2l+3)\alpha^{(2l+3)/2}}{\pi^{\frac{1}{2}}(2l+1)!!}\right]^{\frac{1}{2}},$$

$$G_{n'l'}=\frac{-8\alpha}{2l-1}\left[\frac{2^{l-3}(2l-1)(2l+1)\alpha^{(2l-1)/2}}{\pi^{\frac{1}{2}}(2l-3)!!}\right]^{\frac{1}{2}}\left(1-\frac{2\alpha R^2}{2l+1}\right).$$

DISCUSSION

In the preceding section we have given prescriptions for setting up the wave function for two particles in the same oscillator level in terms of the relative and center-of-mass coordinates. The equations derived carry one as far as the 126 shell. One could, of course, go further but at present there seems no need for this.

When one deals with two particles in different oscillator levels (for example in the region of ${}_{40}\mathrm{Zr}_{50}{}^{90}$ where odd-parity states with $J=4$ or 5 lie fairly low and arise from combining a $p_{\frac{1}{2}}$ and a $g_{9/2}$ particle), the antisymmetrized wave function is not an eigenfunction of H_1 alone and hence one does not have the convenient E_+ operator to work with. In this case one could construct the operator $L_1{}^2+L_2{}^2$, where L^2 is the square of the orbital angular momentum operator. However, as pointed out earlier, it is somewhat tedious to apply this operator when it is expressed in terms of relative and center-of-mass coordinates. Alternatively one could apply the method we have used to obtain the phases of the wave function—namely, expand in a Taylor's series any function of r_1 about the point r_2. However, if one carries out this procedure it is important to note that after the expansion it is, of course, only allowable to replace r_2 by R when one is interested in the behavior of the wave function as $r\rightarrow 0$. If it is desired to retain all powers of r, one has to replace r_2 by $R-r/2$ and carry through some additional Racah algebra.

APPENDIX. SOME SPECIAL EXAMPLES

Some simple and almost trivial examples may help to clarify the method. In order to abbreviate the writing, we shall introduce the notation

$$u_{nl}{}^m=Y_l{}^m(\theta,\phi)R_{nl}(r). \tag{A-1}$$

1. Two nucleons with $n=0$, $l=1$ are coupled to spin 2.—Since the eigenfunction is symmetric in an exchange of the two nucleons, only even values of l can occur in the expansion of the function in terms of R and r. There are only two such terms and we obtain

$$u_{01}{}'(1)u_{01}{}'(2)=\frac{1}{\sqrt{2}}[u_{02}{}^2(R)u_{00}{}^0(r)-u_{00}{}^0(R)u_{02}{}^2(r)]. \tag{A-2}$$

That the coefficients of the two terms differ merely in sign follows from Eq. (16). It is easily checked that the phase is also given correctly and agrees with the value imposed by Eq. (25).

If there exists an interaction potential $V(\mathbf{r}_1-\mathbf{r}_2)=V(\mathbf{r})$ between the nucleons, the energy of the state with $L=2$ can readily be expressed in terms of the moments I_ν of the potential, where

$$I_\nu=\int x^\nu V(\alpha^{-\frac{1}{2}}x)\exp(-x^2/2)x^2dx, \quad (x=\alpha^{\frac{1}{2}}r). \tag{A-3}$$

It is easily seen, by integrating the square of the wave function times $V(r)$ over R and the angles, that only two moments I_0 and I_4 contribute.

Let us note that for r (in which α is replaced by $\alpha/2$) the normalization coefficient for the radial part of the eigenfunction with $n=0$ and any l is

$$\left(\frac{2\alpha^3}{\pi}\right)^{\frac{1}{4}}\frac{\alpha^{l/2}}{[(2l+1)!!]^{\frac{1}{2}}}, \tag{A-4}$$

and for R (where α is replaced by 2α) is

$$\left(\frac{\alpha^3}{2\pi}\right)^{\frac{1}{4}}\frac{2^{l+2}\alpha^{l/2}}{[(2l+1)!!]^{\frac{1}{2}}}. \tag{A-5}$$

It is convenient to use, instead of the moments, the "normalized moments" which are merely the I_ν of Eq. (A-3) multiplied by the square of Eq. (A-4). The factor $\alpha^{l+\frac{3}{2}}$ cancels because $I_{2\nu}$ is defined in terms of x rather than r. The expressions

$$K_{2\nu}=\left(\frac{2}{\pi}\right)^{\frac{1}{2}}\frac{1}{(2\nu+1)!!}I_{2\nu} \tag{A-6}$$

have the property that their value is unity if the potential of interaction is unity. Since the total eigenfunction has to be normalized, one obtains an immediate check on the expression of the interaction energy in terms of the moments, namely, that the sum of the coefficients of the K's must add up to unity.

In the trivial case $(0p)_2{}^2$, one obtains

$$E=\tfrac{1}{2}(K_0+K_4). \tag{A-7}$$

2. Two nucleons with $l=1$, $n=0$ coupling their spins to zero.—The situation in this case is a little less trivial. Again only two terms enter into the expansion, and the ratio of the coefficients can be taken from Eq. (16). Thus

$$\begin{aligned}\frac{1}{\sqrt{3}}\sum_m(-1)^m u_{01}{}^m(1)u_{01}{}^{-m}(2)\\ =-\frac{1}{\sqrt{2}}[u_{10}{}^0(R)u_{00}{}^0(r)-u_{00}{}^0(R)u_{10}{}^0(r)].\end{aligned} \tag{A-8}$$

The phase is also given correctly since in the limit $r\rightarrow 0$, both sides become proportional to $+R^2$. This sign is in agreement with Eq. (25).

The normalized eigenfunctions $u_{10}{}^0$ have the form

$$\begin{aligned}u_{10}{}^0(r)=(4\pi)^{-\frac{1}{2}}(2\alpha^3/\pi)^{\frac{1}{4}}\\ \times 6^{-\frac{1}{2}}(3-\alpha r^2)\exp(-\alpha r^2/4),\end{aligned} \tag{A-9a}$$

$$\begin{aligned}u_{10}{}^0(R)=(4\pi)^{-\frac{1}{2}}(\alpha^3/2\pi)^{\frac{1}{4}}\\ \times 4(6)^{-\frac{1}{2}}(3-4\alpha R^2)\exp(-\alpha R^2).\end{aligned} \tag{A-9b}$$

The normalization coefficient of $u_{00}{}^0(R)$ is $2\sqrt{2}$ times that of $u_{00}{}^0(r)$ [Eq. (A-5)]. Thus it follows that Eq. (A-8) indeed contains only terms proportional to r^2 and R^2, in agreement with Table I.

The expression for the energy of the state with $L=0$ is somewhat more complicated. On squaring the wave function (A-9a), one obtains

$$\frac{1}{4\pi}\left(\frac{2\alpha^3}{\pi}\right)^{\frac{1}{2}}\left\{\tfrac{3}{2}-\frac{1}{3!!}3x^2+\frac{1}{5!!}\tfrac{5}{2}x^4\right\}, \qquad \text{(A-10)}$$

so that

$$\begin{aligned} E&=\tfrac{1}{2}[K_0(1+\tfrac{3}{2})-3K_2+\tfrac{5}{2}K_4] \\ &=\tfrac{1}{4}[5K_0-6K_2+5K_4], \end{aligned} \qquad \text{(A-11)}$$

where again the sum of the coefficients of the K's gives unity.

3. Two nucleons with $n=0$, $l=2$ coupling their spins to $L=4$.—Here the expansion in terms of r and R has the form

$$\begin{aligned} u_{02}{}^2(1)u_{02}{}^2(2)=au_{04}{}^4(R)u_{00}{}^0(r)+bu_{02}{}^2(R)u_{02}{}^2(r) \\ +au_{00}{}^0(R)u_{04}{}^4(r), \end{aligned} \qquad \text{(A-12)}$$

where we have made use of Eq. (16) by equating the coefficients of $u_{04}{}^4(R)u_{00}{}^0(r)$ and $u_{00}{}^0(R)u_{04}{}^4(r)$.

To determine the ratio a/b we operate on this wave function with E_+. This yields the restriction

$$\sqrt{2}a+\sqrt{3}b=0. \qquad \text{(A-13)}$$

Since the function must be normalized, this implies that

$$\begin{aligned} a&=\pm\sqrt{3}/2\sqrt{2}, \\ b&=\mp\tfrac{1}{2}. \end{aligned} \qquad \text{(A-14)}$$

The proper sign is obtained from Eq. (25) which tells us that a must be positive. Thus Eq. (A-12) becomes

$$\begin{aligned} u_{02}{}^2(1)u_{02}{}^2(2)=\frac{1}{2\sqrt{2}}[\sqrt{3}u_{04}{}^4(R)u_{00}{}^0(r) \\ -\sqrt{2}u_{02}{}^2(R)u_{02}{}^2(r) \\ +\sqrt{3}u_{00}{}^0(R)u_{04}{}^4(r)]. \end{aligned} \qquad \text{(A-15)}$$

Since the coupling is still rather simple, one can arrive at the above result without using Racah algebra. Let us consider the case $r_1=r_2=R$, which implies $r=0$. At this point only the first term $au_{04}{}^4(R)u_{00}{}^0(r)$ in Eq. (A-12) is different from zero and is proportional to $\sin^4\Theta e^{4i\Phi}R^4\exp(-\alpha R^2)$. The left-hand side of the equation depends on Θ, Φ, and R in the same way. Thus, as determined from the ratio of the normalization coefficients,

$$2=(2^5/3)a^{\frac{1}{2}} \quad \text{so} \quad a=(3/8)^{\frac{1}{2}}.$$

Since the eigenfunction has to be normalized, the total expression can only be that given by Eq. (A-15), except that the sign of the middle term is undetermined.

That the second term has to be negative can be seen by evaluating the left-hand side of Eq. (A-12) at $\theta_1=0$, $\theta_2=\pi/2$, at which point the product function is zero. In terms of R and r this means that the two azimuthal angles are equal and the other two angles are both equal to $\pi/2$. At this point, then, the intrinsic sign of all three terms is the same. Since the terms must add up to zero, the coefficient of the center term must be negative.

The energy of the state with $L=4$ is then trivially obtained in terms of the moments as

$$E=\tfrac{1}{8}(3K_0+2K_2+3K_4). \qquad \text{(A-16)}$$

It is interesting to note that, in all of the energy expressions considered here, the coefficients of K_0 and $K_{\max}$ have always been the same. This is quite generally true provided we are calculating pairing energies arising from states with no radial nodes. On the other hand, if we were to calculate interaction energies arising from states with radial nodes, the above equality would fail.

Note added in proof.—After this paper was submitted for publication we received preprints from two other groups who have studied this problem [M. Moshinsky, Nuclear Phys. **13**, 104 (1959); A. Arima and T. Terasawa, Progr. Theoret. Phys. (Kyoto) **23**, No. 1 (1960)]. Both of these papers derive recursion relationships between the expansion coefficients $a(n_1l_1; n_2l_2)$, by using properties of the Hermite polynomials.