

# Many-Parameter Wave Functions in the Independent-Particle Model

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It is shown that it is possible to introduce additional parameters into the single-particle wave functions used in estimating, by the Slater method, the lowest eigenvalue of a given Hamiltonian for an  $N$ -nucleon system, without altering the structure of the matrix elements. This is done by associating a different radial parameter with each shell of each  $N$ -particle wave function, subject to certain restrictions. The modification of the matrix elements is given.

## 1. INTRODUCTION

THERE are two well-known methods available of finding upper bounds,  $E_0$ , for the lowest eigenvalue,  $E$ , of the Hamiltonian,  $H$ , of an  $N$ -particle nucleus, when a particular two-body interaction is assumed.

In the variational method, we choose a plausible wave function,  $\Psi_V$  (antisymmetric<sup>1</sup> and normalized), containing a number of variable parameters, with respect to which we minimize the integral

$$\langle \Psi_V^* H \Psi_V \rangle, \quad (1)$$

the minimum value itself being taken as  $E_0$ . The introduction of further parameters into  $\Psi_V$  will generally yield a further decrease of  $E_0$ .

In the method due to Slater in atomic spectroscopy,<sup>2</sup> we begin by choosing an auxiliary Hamiltonian,  $H_A$ , representing the  $N$  nucleons moving independently in an "average" central field,  $V_C = a^{-2}F(r/a)$  (where  $a$  is a constant length).<sup>3</sup> We classify the antisymmetric eigenfunctions,  $\psi$ , of  $H_A$ , by configurations and those "good" quantum numbers which will still be good for  $H$ , as well as by any further quantum numbers which we have reason to believe will be approximately good. We then set up the matrix of  $H$  with respect to  $k$  functions of this set, and find its lowest latent root,  $E_0$ . Adding further functions to the  $k$  already chosen can only cause  $E_0$  to decrease.

How good an approximation  $E_0$  is to  $E$  for a given value of  $k$  (which must usually be small), depends on the choice both of  $H_A$  and of the  $k$  functions,  $\psi^{(1)}, \psi^{(2)}, \dots, \psi^{(k)}$ , used. The quantum numbers for these can largely be obtained from the transformation properties of  $H$  (and of Hamiltonians differing only slightly from  $H$ ), as also (for good quantum numbers) from experimental data. The choice of configurations will be dictated by the ordering of the eigenvalues of  $H_A$ ; i.e.,  $\langle \psi^* H_A \psi \rangle$ . Here the assumption is that this order will be roughly maintained among the corresponding diagonal matrix elements of  $H$ ,  $\langle \psi^* H \psi \rangle$ .

<sup>1</sup> In all  $N$  particles: the use of the isobaric-spin formalism is implied.

<sup>2</sup> J. C. Slater, Phys. Rev. **34**, 1293 (1929).

<sup>3</sup> This functional form of  $V_C$  is chosen in order that the eigenfunctions should (apart from a normalizing factor proportional to  $a^{-3}$ ) depend on  $r$  and on  $a$  only through their ratio. The corresponding eigenvalues vary as  $a^{-2}$ .

The Slater technique can formally be regarded as a special type of variational method:  $\Psi_V$  is taken to be an arbitrary linear combination of the functions  $\psi^{(h)}$  ( $h=1, 2, \dots, k$ ), and the  $k$  coefficients (related by a single normalizing condition, but otherwise independent) serve as variational parameters. If we introduce  $p$  arbitrary parameters into the  $\psi$ 's themselves, the process of finding the minimum latent root of the  $H$  matrix remains equivalent to minimizing the expression (1)—but with respect, now, to all  $\{(k-1)+p\}$  independent parameters—provided only that the orthogonality of the  $\psi$ 's is unaffected by the additional parameters. This last requirement can be satisfied by introducing the parameters into the expression for  $H_A$ , without impairing the status of the  $\psi$ 's as eigenfunctions of a single Hamiltonian; and the one constant  $a$  already included in the definition of  $H_A$  is generally treated as a variation-parameter in this way. But to complicate  $H_A$  beyond this makes it difficult to find its eigenfunctions; and we instead consider a method of introducing additional parameters *directly* into the  $\psi$ 's.

## 2. MODIFIED WAVE FUNCTIONS

We have already seen how to introduce a common parameter,  $a$ , into all the functions: one possible modification would be to allot a different parameter,  $a^{(1)}, a^{(2)}, \dots, a^{(k)}$ , to each of them. But we can go further.

Let us write the spatial eigenfunction with quantum numbers  $n, l, m$  of a single particle in the central field  $V_C$  as

$$R(nl; a) \Theta(lm) \Phi(m),$$

where  $R, \Theta, \Phi$ , depend respectively on the polar coordinates  $r, \theta, \varphi$ , and are separately normalized to unity;  $R$  and  $\Theta$  being real. Then the constant  $a$  will enter only into the radial wave function  $R$ , which alone depends on the form of  $V_C$ . The antisymmetric eigenfunction,  $\psi$ , of  $H_A$ , belonging to a configuration  $\mathfrak{C}$ , where

$$\mathfrak{C} \equiv (n_\alpha l_\alpha)^A (n_\beta l_\beta)^B \dots (n_\gamma l_\gamma)^C, \quad (2)$$

$$(A+B+\dots+C=N),$$

can then always be split into a finite sum of terms, each involving the coordinates  $r_1$  to  $r_N$ , as well as the constant  $a$ , only in the factor

$$R_1(n_\alpha l_\alpha; a) R_2(n_\beta l_\beta; a) \dots R_N(n_\gamma l_\gamma; a), \quad (3a)$$

where  $\lambda, \mu, \dots, \xi$  is some permutation of  $A$   $\alpha$ 's,  $B$   $\beta$ 's,  $\dots$ , and  $C$   $\gamma$ 's.

It is therefore possible to modify the radial wave functions,  $R$ , in each factor of the type (3a), without destroying any of the existing symmetry properties of  $\psi$  with respect to permutations and rotations, provided the same modification is made to all radial wave functions belonging to the same shell (i.e., having the same quantum numbers  $n$  and  $l$ ); for those belonging to different shells are not significantly related. The modification which suggests itself is to associate with each shell in  $\mathfrak{C}$  a different  $a$ : which we can label  $a_\alpha, a_\beta, \dots, a_\gamma$ . Then (3a) is replaced by

$$R_1(n_\lambda l_\lambda; a_\lambda) R_2(n_\mu l_\mu; a_\mu) \cdots R_N(n_\xi l_\xi; a_\xi), \quad (3b)$$

which is a product of  $A$  functions of the type  $R(n_\alpha l_\alpha; a_\alpha)$   $B$  of the type  $R(n_\beta l_\beta; a_\beta)$ ,  $\dots$ , and  $C$  of the type  $R(n_\gamma l_\gamma; a_\gamma)$ . We have now succeeded in introducing additional parameters into  $\psi$  without affecting its previous status as an eigenfunction (belonging to a given eigenvalue) of any operator independent of  $r$ —in particular, it is still antisymmetric; but it has ceased to be an eigenfunction of  $H_A$ .

If we apply the process to each of the  $k$  functions  $\psi^{(h)}$ , we can evidently associate a different set of parameters,  $a_\alpha^{(h)}, a_\beta^{(h)}, \dots, a_\gamma^{(h)}$ , with each wave function. The different  $\psi^{(h)}$  may belong to different configurations  $\mathfrak{C}^{(h)}$  [characterized by a particular set of exponents—some of which may vanish<sup>4</sup>— $A^{(h)}, B^{(h)}, \dots, C^{(h)}$ , in (2)]; but this fact will no longer by itself suffice to ensure the orthogonality which we require of the modified  $\psi^{(h)}$ . The wave functions which cease to be orthogonal are those whose orthogonality as eigenfunctions of  $H_A$  depended exclusively on their configurations differing in a principal quantum number; i.e., on the vanishing of the integral

$$\langle R(nl; a) R(n'l'; a') \rangle, \quad (4)$$

when  $n' \neq n$ ,  $l' = l$ , and  $a' = a$ ; for this fails to vanish when  $a' \neq a$ .

We now reduce the generality with which we can associate different parameters with different shells in each wave function by the following stipulation: If any two among all the shells,  $n_\alpha l_\alpha, n_\beta l_\beta, \dots, n_\gamma l_\gamma$ , represented in the various configurations  $\mathfrak{C}^{(h)}$ , differ only in their principal quantum number, then the identical parameter shall be associated with both those shells wherever they occur, whether in the same or in different wave functions.

Therefore the integral (4), howsoever it arises, will vanish }  
whenever it would originally have done so, i.e., when } (5)  
 $n' \neq n, l' = l.$

Hence, certainly, all previously orthogonal wave functions remain so; for either it is the coefficients of (3) which independently determine orthogonality—

<sup>4</sup> If one of the shells, say  $n_\gamma l_\gamma$ , is not represented in the configuration of a particular function, say  $\psi^{(k)}$ , we need not, of course, define the corresponding parameter  $a_\gamma^{(k)}$ .

and these have not been altered—or the original orthogonality arose from the vanishing of integrals of the type (4), and (5) applies.

### 3. EFFECT ON CALCULATIONS

To show how the use of the modified wave functions affects the results in what we shall always call the “original” case of only the single constant  $a$ , we will assume that the reduction of the matrix elements to sums of radial integrals has, in this case, already been carried out. Methods of doing so—with a general two-body interaction—are well developed.<sup>5</sup>

We consider first a matrix element

$$\langle \psi^* F \psi' \rangle = N \langle \psi^* F_1 \psi' \rangle, \quad (6)$$

where

$$F = \sum_{i=1}^N F_i, \quad F_i = f_i \Lambda_i,$$

$f_i$  being an operator on the coordinate  $r_i$ , and  $\Lambda_i$  an operator on the other coordinates of the  $i$ th particle.  $\psi$  and  $\psi'$  are any members of the modified set  $\psi^{(1)}, \psi^{(2)}, \dots, \psi^{(k)}$ ; possibly both the same.

Expression (6) can be expanded as a finite sum of terms depending on the radial wave functions through a factor of the form

$$\langle R_1(n_\lambda l_\lambda; a_\lambda) f_1 R_1(n_\lambda' l_\lambda'; a_\lambda') \rangle \langle R_2(n_\mu l_\mu; a_\mu) R_2(n_\mu' l_\mu'; a_\mu') \rangle \times \cdots \langle R_N(n_\xi l_\xi; a_\xi) R_N(n_\xi' l_\xi'; a_\xi') \rangle. \quad (7)$$

Here  $n_\lambda l_\lambda, n_\mu l_\mu, \dots, n_\xi l_\xi$  is some permutation of the elements of the configuration,  $\mathfrak{C}$ , of  $\psi$  (and similarly  $n_\lambda' l_\lambda'$ , etc., of  $\mathfrak{C}'$ );  $a_\lambda$  is the parameter associated in  $\psi$  with the shell determined by  $n_\lambda l_\lambda$ , and  $a_\lambda'$  the parameter in  $\psi'$  for the  $n_\lambda' l_\lambda'$  shell. Note that (unless  $\psi' \equiv \psi$ )  $n_\lambda' l_\lambda' \equiv n_\lambda l_\lambda$  does not necessarily imply  $a_\lambda' = a_\lambda$ .

The coefficient of (7) [in the expansion of (6)], which has its original value, must itself be a sum of terms, each containing a factor of the type

$$\langle \Theta_2(l_\mu m_\mu) \Phi_2^*(m_\mu) \Theta_2(l_\mu' m_\mu') \Phi_2(m_\mu') \rangle \times \cdots \langle \Theta_N(l_\xi m_\xi) \Phi_N^*(m_\xi) \Theta_N(l_\xi' m_\xi') \Phi_N(m_\xi') \rangle = \delta(l_\mu, l_\mu') \delta(m_\mu, m_\mu') \cdots \delta(l_\xi, l_\xi') \delta(m_\xi, m_\xi'),$$

so that the whole coefficient contains the factor  $\delta(l_\mu, l_\mu') \cdots \delta(l_\xi, l_\xi')$ . [ $\delta(p, q) \equiv$  Kronecker  $\delta_{pq}$ .] We may therefore, in (7), replace  $l_\mu'$  by  $l_\mu, \dots, l_\xi'$  by  $l_\xi$ ; from which it follows by (5), that we can multiply (7) by  $\delta(n_\mu, n_\mu') \cdots \delta(n_\xi, n_\xi')$  and replace  $n_\mu'$  by  $n_\mu, \dots, n_\xi'$  by  $n_\xi$  elsewhere in the expression.

Thus (7) can be written

$$\delta(n_\mu, n_\mu') \cdots \delta(n_\xi, n_\xi') \times \rho \cdot \langle R_1(n_\lambda l_\lambda; a_\lambda) f_1 R_1(n_\lambda' l_\lambda'; a_\lambda') \rangle, \quad (7a)$$

where

$$\rho = \langle R_2(n_\mu l_\mu; a_\mu) R_2(n_\mu l_\mu; a_\mu') \rangle \cdots \times \langle R_N(n_\xi l_\xi; a_\xi) R_N(n_\xi l_\xi; a_\xi') \rangle;$$

<sup>5</sup> See, for instance, J. P. Elliott, Proc. Roy. Soc. (London) **A218**, 345 (1953).

and, for the original case, (7a) reduces to

$$\delta(n_\mu, n'_\mu) \cdots \delta(n_\xi, n'_\xi) \langle R_1(n_\lambda l_\lambda; a) f_1 R_1(n'_\lambda l'_\lambda; a) \rangle. \quad (7b)$$

Since (7b) vanishes identically only when (7a) does, the modified calculation can be deduced from the original one by replacing (7b) by (7a), without introducing any additional terms. (We are assuming that the original coefficient of every integral of the type  $\langle R_1 f_1 R_1' \rangle$  in (7b) has been calculated, even though a particular integral might happen to be zero.) Dropping the unnecessary particle-suffices, we can formalize this into the following rule for the modified calculation:

In the original case, expand (6) as a sum of terms

$$A \cdot \langle R(n_\lambda l_\lambda; a) f R(n'_\lambda l'_\lambda; a) \rangle,$$

and replace each such term by

$$A \cdot \rho \cdot \langle R(n_\lambda l_\lambda; a_\lambda) f R(n'_\lambda l'_\lambda; a'_\lambda) \rangle,$$

where

$$\rho = \langle R(n_\mu l_\mu; a_\mu) R(n_\mu l_\mu; a'_\mu) \rangle \cdots \langle R(n_\xi l_\xi; a_\xi) R(n_\xi l_\xi; a'_\xi) \rangle;$$

the values of  $n_\mu l_\mu, \dots, n_\xi l_\xi$  being determined by the requirement that  $n_\lambda l_\lambda, n_\mu l_\mu, \dots, n_\xi l_\xi$  should constitute a re-arrangement of  $\mathfrak{E}$ , and  $n'_\lambda l'_\lambda, n'_\mu l'_\mu, \dots, n'_\xi l'_\xi$  a re-arrangement of  $\mathfrak{E}'$ .<sup>6</sup>

By a precisely similar argument, we see that we can perform the modified calculation of a matrix element

$$\langle \psi^* G \psi \rangle = \frac{1}{2} N(N-1) \langle \psi^* G_{12} \psi \rangle, \quad (8)$$

where

$$G = \sum_{i>j=1}^N G_{ij}, \quad G_{ij} = g_{ij} \Gamma_{ij},$$

( $g_{ij}$  being an operator on  $r_i$  and  $r_j$ , and  $\Gamma_{ij}$  an operator on the other coordinates of the  $i$ th and  $j$ th particles) by the following rule:

In the original case, expand (8) as a sum of terms

$$B \cdot \langle R_1(n_\lambda l_\lambda; a) R_2(n_\mu l_\mu; a) g_{12} R_1(n'_\lambda l'_\lambda; a) R_2(n'_\mu l'_\mu; a) \rangle,$$

and replace each such term by

$$B \cdot \sigma \cdot \langle R_1(n_\lambda l_\lambda; a_\lambda) R_2(n_\mu l_\mu; a_\mu) g_{12} R_1(n'_\lambda l'_\lambda; a'_\lambda) R_2(n'_\mu l'_\mu; a'_\mu) \rangle, \quad (9)$$

where

$$\sigma = \langle R(n_\nu l_\nu; a_\nu) R(n_\nu l_\nu; a'_\nu) \rangle \cdots \langle R(n_\xi l_\xi; a_\xi) R(n_\xi l_\xi; a'_\xi) \rangle;$$

the values of  $n_\nu l_\nu, \dots, n_\xi l_\xi$  being determined by the requirement that, together with  $n_\lambda l_\lambda$  and  $n_\mu l_\mu$ , they should form a re-arrangement of  $\mathfrak{E}$ , while, together with  $n'_\lambda l'_\lambda$  and  $n'_\mu l'_\mu$ , they must form a re-arrangement of  $\mathfrak{E}'$ .<sup>7</sup>

Since  $H$  can always be expanded as a sum of operators of the type  $F$  and  $G$ , our two rules determine the calculation of its matrix with respect to the  $k$  modified wave functions.

<sup>6</sup> This double condition restricts the functions  $\psi'$ , for which the matrix element (6) does not vanish, to those whose configurations differ in at most one state from  $\psi$ .

<sup>7</sup> This double condition restricts the functions  $\psi'$ , for which the matrix element (8) does not vanish, to those whose configurations differ in at most two states from  $\psi$ .

#### 4. SPHERICAL OSCILLATOR WAVE FUNCTIONS

As an illustration, we give the very simple form which the constituents of  $\rho$  and  $\sigma$  take when the auxiliary potential is that of a three-dimensional harmonic oscillator; i.e.,  $V_C = (\hbar^2/2Ma^2)(r/a)^2 = \frac{1}{2}M\omega^2 r^2$ , where  $M$  denotes the nucleon-mass and  $2\pi/\omega$  the period of the corresponding classical oscillator.

The energy of the single-particle eigenstate with quantum numbers  $n$  and  $l$  is<sup>8</sup>  $(2n-l-\frac{1}{2})\hbar\omega$ . The radial wave function of the *lowest* eigenstate with a given  $l$ , i.e., of the state (with energy  $(l+\frac{3}{2})\hbar\omega$ ) for which  $n=l+1$ , is  $K_l a^{-\frac{1}{2}}(r/a)^l \exp[-\frac{1}{2}(r/a)^2]$ , where  $K_l$ , determined by the normalizing condition, depends only on  $l$ . In this case (with  $n=l+1$ ),  $\langle R(nl; a) R(nl; a') \rangle = \{2aa'/(a^2+a'^2)\}^{l+\frac{1}{2}}$ , or  $|\sin^{l+\frac{1}{2}}\kappa|$ , where  $a'/a = \tan\frac{1}{2}\kappa$ .

Corresponding expressions for  $n>l+1$  will not be required in practice, since the configurations of the  $k$  functions used will always include one in which any given value of  $l$  that is represented at all among them occurs in association with the lowest possible value of  $n$ , viz.,  $l+1$ ; and if any other shell associates that  $l$  with some higher  $n$ , the identical-parameter stipulation comes into play.

A formula by which the rather complex integrals of the type occurring in (9) can be calculated in the present case is given elsewhere.<sup>9</sup>

#### 5. CONCLUDING REMARKS

The effect of the modification is to add a "synthetic" mixture of states to the  $k$  originally chosen.

We can expand a radial wave function of given parameter in terms of all those, associated with the same orbital angular momentum, of any other parameter; i.e.,

$$R(n'l; a') = \sum_{n=l+1}^{\infty} c_n R(nl; a),$$

where the  $c_n$  do not depend on  $r$ .<sup>10</sup> It follows that the variation of the parameter of a particular shell ( $n_\lambda l_\lambda$ ), within a particular eigenstate of  $H_A$ , is important just in so far as—in building up the correct wave function—those eigenstates are important whose configurations associate  $l_\lambda$  with other principal quantum numbers than  $n_\lambda$ . The identical-parameter stipulation allows the parameter to vary just when such configurations as these are not represented among the eigenstates originally considered.

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<sup>8</sup> We define  $n$  to be  $(\bar{n}+l+1)$ , as in atomic spectroscopy [rather than  $(\bar{n}+1)$ ]; where  $\bar{n}$  is the number of finite nodes of the function  $R$  for  $r>0$ .

<sup>9</sup> E. H. Kronheimer, Phys. Rev. **90**, 1003 (1953); Phys. Rev. **91**, 1580 (1953).

<sup>10</sup> They are, of course, the integrals (4) with  $l'=l$ .