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Nuclear Spectroscopy

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XV CORSO

a cura di G. RACAH
Direttore del Corso

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Spettroscopia Nucleare

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Prolusione al Corso.

G. Racah

Direttore del Corso

When I was told that, according to tradition, I would have to deliver the opening address at this gathering, I glanced at the addresses of my predecessors in order to discover what that tradition was.

I found that there were two categories of opening addresses: if the speaker were an Italian, it was his main task to thank the foreign teachers who had agreed to participate in the courses; if he were a foreigner, his function was to thank the Società Italiana di Fisica which had organized the Course.

Being at the same time both an Italian and a foreigner, it is my very pleasant duty to thank both parties. And I should like to start by expressing our gratitude to the Ente Villa Monastero, our host in this magnificent spot on the Lake of Como, in this beautiful building which was once the residence of Marco and Rosa De Marchi who donated it for the purpose of furthering the development of science.

Next, I should like to thank the Società Italiana di Fisica, and particularly its President, Professor POLVANI, who organized this Course in the same exemplary manner as he has organized all the preceding courses. I arrived only yesterday, but I have already had time to see that everything is in perfect order.

The fact that I have been asked to serve as Director of the School precisely this year is cause for particular emotion as far as I am concerned, because this is the first time that the School of Varenna has been named after ENRICO FERMI, my own unforgettable teacher and the teacher of all of us. It is appropriate indeed that the School should bear his name, not only for the obvious reasons but also because the lectures he delivered here, in this room, were the last lectures of his life.

Since I am more familiar with the Mathematics than with the Physics of Nuclear Spectroscopy, it was not an easy task for me to organize the programme for this course; however, I did my best, which means that I tried to find the best. I. Talmi and B. Mottelson will lecture on Nuclear Structure. They are typical representatives of two different approaches: the independent particle model and the collective model. I hope that the clash between these two opposite points of view will be one of the most interesting features of this course.

G. Alaga and G. Morpurgo will lecture on nuclear radiations, and J. Goldstone will deal with the most recent developments in the theory of Nuclear Matter.

I hope that many of the participants will contribute to the discussion on their subjects by recounting their own particular experiences in order to supplement the official lectures.

To the lecturers I wish to express my deep gratitude, and to the participants I extend a warm welcome to this School.

Mathematical Techniques.

G. Racah

Department of Physics, Hebrew University of Jerusalem

1. – Coupling of angular momenta.

The first task of the theoretical nuclear spectroscopist is to calculate the energy levels of the nuclei; the second task is to calculate other properties of the nuclear states, like magnetic moments, quadrupole moments, transition probabilities, etc. In these lectures we shall mainly concentrate on the energy levels; some of the other lectures will deal with the other properties.

The official method for calculating energy levels both in atomic spectroscopy and in nuclear spectroscopy is first to write down the Schrödinger equation,

$$H\psi = E\psi\,,$$

and then to solve it. In atomic spectroscopy the first step is very easy, but the second step is very difficult if we have an atom with 10, 20, or 102 electrons. In nuclear spectroscopy even the first step is very difficult, because we do not know very much about the nuclear forces, and therefore we cannot write down the Hamiltonian. The difference between the two cases is not so fundamental as it seems at first sight, because, if we cannot solve the Schrödinger equation, the fact that we can write it down is not very helpful.

Since it is impossible to solve directly the Schrödinger equation, the practical method for calculating energy levels in atomic spectroscopy is to take an orthonormal set of functions

$$\psi_a,\ \psi_b,\ \psi_c\,,\ \dots \tag{1}$$

which are as near as possible to the eigenfunctions of the Schrödinger equation to calculate the matrix elements

$$(a|H|b) = \int \overline{\psi}_a H \psi_b \,\mathrm{d}\tau\,, \tag{2}$$

and then to proceed by approximation methods.

In nuclear spectroscopy even this program is difficult to execute, because we do not know the Hamiltonian and we know very little about the functions. But if we know some properties of the Hamiltonian and some features of the functions (1) it is possible to get some information about the matrix elements. I would therefore like to define the task of the theoretical nuclear spectroscopist to say as much as possible about the matrix elements (2) by assuming as less as possible about the Hamiltonian and about the functions (1).

We shall start by looking what we can say about the eigenfunctions and how we can build the orthonormal set (1). The first thing we know from the experiment is that the nucleons are ordered in shells. Mathematically this means that if we have a single nucleon outside closed shells, the state of this nucleon will be characterized by a radial quantum number n, an azimuthal quantum number l, a magnetic quantum number m_l and a spin quantum number m_s. Moreover we know from the experiment that, except for very light nuclei, the orbital momentum is strongly coupled with the spin so that the actual quantum numbers will be $nljm$. States with the same quantum numbers nlj will be said to belong to the same shell. In the following we shall forget about n and l, and characterize in general a shell by the sole quantum number j, and the states of a nucleon by the symbol $|jm)$.

If we have two nucleons outside closed shells, one in a shell j_a and the other in a shell j_b any state of the two particle system will be a superposition of the states

$$|j_a m_a)|j_b m_b) = |j_a m_a j_b m_b)\,, \tag{3}$$

If we want to classify the states of this system according to the eigenvalues of the total angular momentum, we have to replace the states (3) with the states

$$|j_a j_b J M) = \sum_{m_a m_b} |j_a m_a j_b m_b)(j_a m_a j_b m_b|j_a j_b J M)\,. \tag{4}$$

The coefficients of the transformation on the right-hand side of (4) are called the Wigner coefficients. These coefficients have many important properties which are assumed to be well known; we shall only remember here the symmetry property

$$(j_a m_a j_b m_b|j_a j_b J M) = (-1)^{j_a+j_b-J}(j_b m_b j_a m_a|j_b j_a J M)\,, \tag{5}$$

which is of particular interest for us.

In the case of three nucleons, the building of eigenfunctions of the total angular momentum is not unique, and depends on the choice of a particular coupling scheme. If the first two nucleons are coupled first, the eigenfunctions will be

$$(6)\qquad |j_a j_b j_c J_{ab} J M) = \\ = \sum_{m_a m_b m_c M_{ab}} |j_a m_a j_b m_b j_c m_c)(j_a m_a j_b m_b | j_a j_b J_{ab} M_{ab})(J_{ab} M_{ab} j_c m_c | J_{ab} j_c J M);$$

if the last two sets are coupled first the eigenfunctions will be

$$(7)\qquad |j_a j_b j_c J_{bc} J M) = \\ = \sum_{m_a m_b m_c M_{bc}} |j_a m_a j_b m_b j_c m_c)(j_b m_b j_c m_c | j_b j_c J_{bc} M_{bc})(j_a m_a J_{bc} M_{bc} | j_a J_{bc} J M).$$

The first nucleon may also be coupled with the third one.

From the mathematical point of view the three coupling schemes are completely equivalent. The eigenfunctions of each scheme constitute a complete set of orthogonal eigenfunctions and may also be expressed as linear combinations of the eigenfunctions of another scheme. The orthogonal substitution which connects (6) and (7) is

$$(8)\qquad (j_a j_b j_c J_{ab} J | j_a j_b j_c J_{bc} J) = \\ = \sum_{m_a m_b m_c M_{ab} M_{bc}} (J_{ab} j_c J M | J_{ab} M_{ab} j_c m_c)(j_a j_b J_{ab} M_{ab} | j_a m_a j_b m_b) \cdot \\ \cdot (j_b m_b j_c m_c | j_b j_c J_{bc} M_{bc})(j_a m_a J_{bc} M_{bc} | j_a J_{bc} J M).$$

The elements of this substitution can be calculated to be

$$(9)\qquad (j_a j_b j_c J_{ab} J | j_a j_b j_c J_{bc} J) = (-1)^{j_a + j_b + j_c + J} \sqrt{(2J_{ab}+1)(2J_{bc}+1)}\, \overline{W} \begin{pmatrix} j_a & j_b & J_{ab} \\ j_c & J & J_{bc} \end{pmatrix},$$

where the function $\overline{W}$ or « six-j-symbol » has the expression

$$(10)\quad \overline{W}\begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix} = \sqrt{\frac{(a+b-c)!(a-b+c)!(b+c-a)!(d+e-c)!(d-e+c)!}{(a+b+c+1)!(d+e+c+1)!}} \cdot \\ \cdot \sqrt{\frac{(e+c-d)!(d+b-f)!(d-b+f)!(b+f-d)!(a+e-f)!(a-e+f)!(e+f-a)!}{(d+b+f+1)!(a+e+f+1)!}} \cdot \\ \cdot \sum_q \frac{(-1)^q (q+1)!}{(q-a-b-c)!(q-d-e-c)!(q-d-b-f)!(q-a-e-f)!} \cdot \\ \cdot \frac{1}{(a+b+d+e-q)!(a+c+d+f-q)!(b+c+e+f-q)!}.$$

From the physical point of view the three coupling schemes are not equivalent, but describe different situations. States of a three-nucleon system, which are eigenstates of the energy, do not belong to any of those coupling schemes, because the matrix of the interaction between the nucleons is not diagonal in any of the three schemes. However if the interaction between the nucleons in the states a and b is much stronger than the interaction with the third one, the energy eigenstates will be very near to the states (6). The state of the pair a, b which is characterized by the quantum number J_{ab} is called the parent of the state (6).

2. - **Antisymmetrization.**

According to the Pauli principle the eigenfunctions of identical nucleons must be antisymmetric with respect to permutations of the coordinates. We shall indicate all the coordinates of the n-th nucleon by the numeral n, and the eigenfunctions, representing eigenstates in terms of coordinates, by brackets.

In this notation eq. (4) becomes

$$(12|j_aj_bJM) = \sum_{m_am_b} (1|j_am_a)(2|j_bm_b)(j_am_aj_bm_b|j_aj_bJM)\,. \tag{11}$$

Permutation of the particle coordinates yields the eigenfunctions

$$(21|j_aj_bJM) = \sum_{m_am_b} (2|j_am_a)(1|j_bm_b)(j_am_aj_bm_b|j_aj_bJM)\,, \tag{12}$$

and using the symmetry property (7) these eigenfunctions become

$$(-1)^{j_a+j_b-J} \sum_{m_am_b} (2|j_am_a)(1|j_bm_b)(j_bm_bj_am_a|j_bj_aJM) = (-1)^{j_a+j_b-J}(12|j_bj_aJM)\,. \tag{13}$$

Therefore

$$(21|j_aj_bJM) = (-1)^{j_a+j_b-J}(12|j_bj_aJM)\,. \tag{14}$$

In the particular case $j_a = j_b = j$ the eigenfunction on the right side of (14) coincides with (11), and therefore $(12|j^2JM)$ is symmetric or antisymmetric according to the parity of $2j - J$. In the general case $j_a \neq j_b$ the eigenfunction on the right side of (14) is different from, and actually orthogonal to (11), and neither of them has a definite symmetry. We may, however construct antisymmetric eigenfunctions by taking an antisymmetric combination of (11) and (14). We indicate antisymmetric eigenfunctions by the notation $(12\}j_aj_bJM)$, and write

$$(12\}j_aj_bJM) = \frac{1}{\sqrt{2}}[(12|j_aj_bJM) - (21|j_aj_bJM)]\,, \tag{15}$$

or

$$(15') \qquad (12]\}j_aj_bJM) = \frac{1}{\sqrt{2}}\left[(12\,|\,j_aj_bJM) - (-1)^{j_a+j_b-J}(12\,|\,j_bj_aJM)\right],$$

where the factor $1/\sqrt{2}$ preserves the normalization.

Notice that for $j_a = j_b = j$ the right side of these equations would vanish for odd J and would have the wrong normalization for even J. In this last case we must write

$$(16) \qquad (12]\}j^2JM) = (12\,|\,j^2JM)\,, \qquad (J \text{ even});$$

$(12]\}j^2JM)$ does not exist for odd J.

The equation

$$(17) \qquad (12]\}j_aj_bJM) = -(-1)^{j_a+j_b-J}(12]\}j_bj_aJM)\,,$$

holds independently of whether j_a coincides with j_b.

In the case of three nucleons, if $j_a \neq j_b \neq j_c$, the analog of (15) is

$$(18) \qquad (123]\}j_aj_bj_cJ_{ab}JM) = \frac{1}{\sqrt{6}}\left[(123\,|\,j_aj_bj_cJ_{ab}JM) - (213\,|\,j_aj_bj_cJ_{ab}JM) + \right.$$
$$\left. + (231\,|\,j_aj_bj_cJ_{ab}JM) - (321\,|\,j_aj_bj_cJ_{ab}JM) + (312\,|\,j_aj_bj_cJ_{ab}JM) - (132\,|\,j_aj_bj_cJ_{ab}JM)\right].$$

For $j_a = j_b = j_c = j$ the six terms on the right side of this equation are no more orthogonal; and therefore (18) is no more normalized. In order to construct antisymmetric normalized eigenfunctions, we start from the eigenfunctions

$$(19) \qquad (12\}3\,|\,j^2J_0, jJM) = \sum_{M_0m}(12]\}j^2J_0M_0)(3\,|\,jm)(J_0M_0jm\,|\,J_0jJM) \qquad (J_0 \text{ even}),$$

which are antisymmetric only with respect to the first two nucleons, and apply to them the « antisymmetrizator » A defined by

$$(20) \qquad A(12\}3\,|\,j^2J_0, jJM) =$$
$$= \tfrac{1}{3}\left[(12\}3\,|\,j^2J_0, jJM) + (23\}1\,|\,j^2J_0, jJM) + (31\}2\,|\,j^2J_0, jJM)\right].$$

We reduce now all three terms on the right side to the same coupling scheme as the first one. The second term is

$$(21a) \qquad (23\}1\,|\,j^2J_0, jJM) =$$
$$= \sum_{J'}(-1)^{J_0}\sqrt{(2J_0+1)(2J'+1)}\;\overline{W}\begin{pmatrix} j & j & J_0 \\ j & J & J' \end{pmatrix}(123\,|\,j^2J', jJM)\,,$$

and the third term is

(21b)
$$(31\}2\,|\,j^2J_0,\,jJM) =$$
$$= \sum_{J'} (-1)^{J'} \sqrt{(2J_0+1)(2J'+1)}\;\overline{W}\begin{pmatrix} j & j & J_0 \\ j & J & J' \end{pmatrix} (123\,|\,j^2J',\,jJM)\,.$$

The contributions of these two terms are equal if $J' - J_0$ is even, and opposite if $J' - J_0$ is odd. Since J_0 is itself even, the expansion of (20) contains only terms with J' even. Introducing (21a) and (21b) into (20) we get

(22)
$$A(12\}3\,|\,j^2J_0,\,jJM) = \sum_{J'} (12\}3\,|\,j^2J',\,jJM)(J'\,|\,A(J)\,|\,J_0)\,, \qquad (J',\,J_0 \text{ even})\,,$$

where

(23)
$$(J'\,|\,A(J)\,|\,J_0) =$$
$$= (J_0\,|\,A(J)\,|\,J') = \frac{1}{3}\,\delta_{J'J_0} + \frac{2}{3}\sqrt{(2J_0+1)(2J'+1)}\;\overline{W}\begin{pmatrix} j & j & J_0 \\ j & J & J' \end{pmatrix}.$$

No antisymmetric eigenfunctions of three nucleons exist for those values of J for which every $(J'\,|\,A(J)\,|\,J_0)$ vanishes. When these eigenfunctions exist, the functions (22) are still not normalized and have to be divided by $\sqrt{N_{J_0}(J)}$, where

(24)
$$N_{J_0}(J) = \sum_{J'} (J'\,|\,A(J)\,|\,J_0)^2\,.$$

Since the antisymmetrizator A is normalized in such a way that it leaves invariant a function which is already antisymmetric, it satisfies the equation

(25)
$$A^2 = A\,,$$

from which we get that

(26)
$$N_{J_0}(J) = (J_0\,|\,A(J)\,|\,J_0)\,.$$

Therefore the functions

(27)
$$(123\}\,j^3(J_0)JM) = (J_0\,|\,A(J)\,|\,J_0)^{-\frac{1}{2}} \sum_{J'} (12\}3\,|\,j^2J',\,jJM)(J'\,|\,A(J)\,|\,J_0)\,,$$

are normalized antisymmetric eigenfunctions of the configuration j^3.

It should be emphasized that for different values of J_0 these eigenfunctions are not orthogonal or even linearly independent. In many cases they are actually identical. This fact is easy to understand, because eq. (25) shows that the antisymmetrizator A is a projection operator, *i.e.* an operator which transforms every function into its orthogonal projection in the subspace of the antisymmetric functions. It is then evident that by projecting into a subspace a complete set of orthogonal vectors of the whole space, we get a set of vectors which are linearly dependent. This set of linearly dependent functions can easily be replaced with an orthogonal set by the well known orthogonalization procedures of vector algebra. These orthogonal antisymmetric eigenfunctions are, in general, no longer characterized by the quantum numbers J_0, but by different quantum numbers α. A general antisymmetric eigenfunction has then the form

$$(28)\qquad (123|\}\, j^3\alpha JM) = \sum_{J'} (12\}3\,|\,j^2J', jJM)(j^2J', j, J|\}\, j^3\alpha J)\,,$$

and the coefficients of this expansion satisfy the equation

$$(29)\qquad \sum_{J'} (J_0\,|\,A(J)\,|\,J')(j^2J', j, J|\}\, j^3\alpha J) = (j^2J_0, j, J|\}\, j^3\alpha J)\,,$$

which identifies them as eigenvectors of the matrix A corresponding to the eigenvalue 1.

In conclusion the states (19) have a well defined parent, but are not antisymmetric, the states (27) and (28) are antisymmetric but have no well defined parent. Therefore the coefficients of the expansion (28) are called « coefficients of fractional parentage ».

The estension to antisymmetric functions of r nucleons belonging to the same shell is almost immediate. These eigenfunctions will be obtained by starting from eigenfunctions $(12\,...\,r-1\}r\,|\,j^{r-1}\alpha_0J_0, j, JM)$, which are antisymmetric only with respect to the first $r-1$ nucleons, and by taking those linear combinations of them,

$$(30)\quad (12\,...\,r|\}\, j^r\alpha JM) = \sum_{\alpha'J'} (12\,...\,r-1\}r\,|\,j^{r-1}\alpha'J', j, JM)(j^{r-1}\alpha'J', j, J|\}\, j^r\alpha J)\,,$$

which are antisymmetrical with respect to all the nucleons. The coefficients of these linear combinations will satisfy the equations

$$(31)\qquad \sum_{\alpha'J'} (\alpha_0J_0\,|\,A(J)\,|\,\alpha'J')(j^{r-1}\alpha'J', j, J|\}\, j^r\alpha J) = (j^{r-1}\alpha_0J_0, j, J|\}\, j^r\alpha J)\,,$$

where

$$(32)\qquad (\alpha'J'\,|\,A(J)\,|\,\alpha_0J_0) = (\alpha_0J_0\,|\,A(J)\,|\,\alpha'J') =$$
$$= \frac{1}{r}\delta_{\alpha'\alpha_0}\delta_{J'J_0} + \frac{r-1}{r}(-1)^{J'+J_0}\sum_{\alpha''J''}\sqrt{(2J_0+1)(2J'+1)}\;\overline{W}\begin{pmatrix} j & J'' & J' \\ j & J & J_0 \end{pmatrix}\cdot$$
$$\cdot(j^{r-1}\alpha'J'\{|\,j^{r-2}\alpha''J'', j, J')(j^{r-2}\alpha''J'', j, J_0|\}\, j^{r-1}\alpha_0J_0)\,.$$

3. – The energy matrix. Part I.

After having seen how to build wave functions of a nuclear system which may be hoped to be fairly near to the real eigenfunctions, we can go back to the problem of calculating the energy matrix. In the shell-model approximation we write the Hamiltonian as

$$H = \sum_i \left[T_i + U(r_i) + \zeta_i(s_i \cdot l_i)\right] + \sum_{i<k} V_{ik}\,, \tag{33}$$

where the summation is extended only to the particles outside closed shells, T_i is the kinetic energy of the i-th particle, $U(r_i)$ its potential energy in the field produced by the closed shells, and V_{ik} the interaction between the particles i and k.

If we assume that in the zero-th approximation the external particles move independently in the central field $U(r)$, the single-particle functions will be eigenfunctions of

$$H_i = T_i + U(r_i) + \zeta_i(s_i \cdot l_i)\,, \tag{34}$$

corresponding to the eigenvalues ε_i, and the problem will reduce to the calculation of the matrix of the last term of (33).

For a system of two particles outside closed shells we have to calculate the matrix of V_{12}. Since the single-particle functions are the product of a radial function $(1/r)R_{nl}(r)$ times a function of the angular and spin coordinates, if $V_{12} = V(r_{12})$ with $r_{12}^2 = r_1^2 + r_2^2 - 2r_1r_2\cos\omega_{12}$, we shall separate also here the radial dependence from the angular dependence by expanding $V(r_{12})$ into a series of Legendre polynomials of $\cos\omega_{12}$.

$$V(r_{12}) = \sum_k v_k(r_1, r_2)P_k(\cos\omega_{12})\,. \tag{35}$$

Then the matrix elements of $V(r_{12})$ get the form

$$\begin{aligned}(n_al_aj_an_bl_bj_bJM\,|\,V(r_{12})\,|\,n_cl_cj_cn_dl_dj_dJM) = \\ = \sum_k R^k(n_al_an_bl_b, n_cl_cn_dl_d)(l_aj_al_bj_bJM\,|\,P_k(\cos\omega_{12})\,|\,l_cj_cl_dj_dJM)\,,\end{aligned} \tag{36}$$

where the R^k are the generalized Slater integrals

$$R^k(n_al_an_bl_b, n_cl_cn_dl_d) = \iint R_{n_al_a}(r_1)R_{n_bl_b}(r_2)v_k(r_1, r_2)R_{n_cl_c}(r_1)R_{n_dl_d}(r_2)\,\mathrm{d}r_1\,\mathrm{d}r_2\,. \tag{37}$$

The calculation of the matrix elements of $P_k(\cos\omega_{12})$ is a purely algebrical problem, which can be solved exactly, because the expressions of the Legendre polynomials and of the angular eigenfunctions are well known. The calculation of the generalized Slater integrals requires the knowledge of the $v_k(r_1, r_2)$ and of the radial eigenfunctions. In atomic spectroscopy the $v_k(r_1, r_2)$ are very well known, while in nuclear spectroscopy they are almost unknown. But also in this case the difference is not very fundamental, because in both cases the radial eigenfunctions are known only very roughly, and if in a product of five functions four are known only roughly, the knowledge of the fifth is not very decisive.

However, in atomic spectroscopy we can manage to proceed without knowing the radial eigenfunctions. For the first approximation we need only the diagonal elements of the interaction matrix, which for two equivalent electrons in *LS*-coupling, are

$$((nl)^2LM\,|\,e^2/r_{12}\,|\,(nl)^2LM) = \sum_k R^k(nlnl,\,nlnl)(l^2\,LM\,|\,P_k(\cos\omega_{12})\,|\,l^2LM)\,. \tag{38}$$

Since the matrix elements of $P_k(\cos\omega_{12})$ are different from zero only if k is even and not larger than $2l$, we can express the theoretical energies of $2l+1$ differential levels by only $l+1$ Slater integrals, and it is possible to compare theory and experiment without actually calculating the Slater integrals. The results of this comparison show that in many cases the agreement is qualitatively good, but quantitatively unsatisfactory, and we can say that even in atomic spectroscopy the first approximation of the pure shell model does not give satisfactory results.

In nuclear spectroscopy even a comparison of this kind is impossible because, as we have already heard from Dr. GOLDSTONE, the nuclear forces do not depend only on the distance between the nucleons, but also on the spin orientations and on the symmetry of the eigenfunctions. The number of independent Slater integrals is therefore multiplied by four and becomes much larger than the number of levels in a two-particle configuration.

The results are much more interesting and satisfactory in configurations with three or more particles in the same shell.

For a three-particle configuration the matrix of $V_{12}+V_{13}+V_{23}$ may be easily obtained from $(j^2J\,|\,V_{12}\,|\,j^2J)$ by the formula

$$(j^3\alpha J\,|\,V_{12}+V_{13}+V_{23}\,|\,j^3\alpha' J) = \\ = 3\sum_{J'}(j^3\alpha J\,|\,j^2J',\,j,\,J)(j^2J'\,|\,V_{12}\,|\,j^2J')(j^2J',\,j,\,J\,|\,j^3\alpha' J)\,. \tag{39}$$

For more than three particles we have two equivalent methods for calculating the matrix

$$(j^n\alpha J\,|\sum V_{ik}\,|\,j^n\alpha' J)\,. \tag{40}$$

The first method is a recursion method, and calculates the matrix for j^n from the matrix for j^{n-1}:

$$(41)\qquad (j^n\alpha J|\sum V_{ik}|j^n\alpha' J) =$$

$$= \frac{n}{n-2}\sum_{\alpha_1\alpha_1' J_1}(j^n\alpha J\{\!|j^{n-1}\alpha_1 J_1, j, J)(j^{n-1}\alpha_1 J_1|\sum V_{ik}|j^{n-1}\alpha_1' J_1)(j^{n-1}\alpha_1' J_1, j, J|\!\}j^n\alpha' J)\,;$$

the factor $n/(n-2)$, which appears in this formula, is the ratio between the numbers of pairs in the configurations j^n and j^{n-1}.

The second method seems a more direct method, but it requires the knowledge of the eigenfunctions of j^n as linear combinations of the eigenfunctions of $j^{n-2}j^2$:

$$(42)\qquad (12\,...\,n|\!\}j^n\alpha JM) =$$

$$= \sum_{\alpha_1 J_1 J_2}(12\,...\,n-2\}n-1\;n|j^{n-2}\alpha_1 J_1, j^2 J_2, JM)(j^{n-2}\alpha_1 J_1, j^2 J_2, J|\!\}j^n J)\,.$$

The coefficients of this expansion, which may be called coefficients of fractional grand-parentage, are given by the formula

$$(43)\qquad (j^{n-2}\alpha_1 J_1, j^2 J_2, J|\!\}j^n\alpha J) = \sum_{\alpha' J'}(j^{n-2}\alpha_1 J_1, j, J'|\!\}j^{n-1}\alpha' J')\,\cdot$$

$$\cdot\,(j^{n-1}\alpha' J', j, J|\!\}j^n\alpha J)(-1)^{2j+J_1+J}\sqrt{(2J'+1)(2J_2+1)}\;\overline{W}\begin{pmatrix} J_1 & j & J' \\ j & J & J_2 \end{pmatrix},$$

and may be used for calculating the matrix (40):

$$(44)\qquad (j^n\alpha J|\sum V_{ik}|j^n\alpha' J) =$$

$$= \tfrac{1}{2}n(n-1)\sum_{\alpha_1 J_1 J_2}(j^n\alpha J\{\!|j^{n-2}\alpha_1 J_1, j^2 J_2, J)(j^2 J_2|V_{12}|j^2 J_2)(j^{n-2}\alpha_1 J_1, j^2 J_2, J|\!\}j^n\alpha' J)\,.$$

For practical calculations the first method is more convenient, because the calculation of the coefficients (43) is rather cumbersome; but on the other hand eq. (44) has the advantage of being a closed formula and not a recursion formula, and is therefore more convenient for proving general properties of the matrix (40).

In atomic spectroscopy the agreement between theory and experiment for the configurations l^n is similar to that for the configurations l^2 which means not very satisfactory; but if in eq. (44) we substitute the theoretical expressions of $(l^2L_2|V_{12}|l^2L_2)$ with the experimental values $E(l^2L_2)$, or more generally if we consider the values of $(l^2L_2|V_{12}|l^2L_2)$ as freely adjustable parameters, the agreement is very much improved. Of course in a formula with freely adjustable parameters, an increase of the number of parameters always improves the agreement, but the question is how much the agreement is improved. For instance, in the configurations $3d^2$ we cannot get a good fitting of four terms with three adjustable parameters, while in the configurations $3d^4$ and $3d^5$ we can very well fit twelve or more terms with only five parameters.

In nuclear spectroscopy the substitution of $(j^2J\,|\,V_2\,|\,j^2J)$ with $E(j^2J)$ does not increase the number of parameters, and even decreases it. Moreover it has the advantage that it does not require any assumption about the shape, spin dependence and symmetry dependence of the nuclear forces. The agreement with the experimental data, in the few cases where it was possible to check it, seems also to be good, as we shall hear later in detail from Dr. TALMI.

We want therefore to discuss why the substitution of $(j^2J\,|\,V_{12}\,|\,j^2J)$ with $E(j^2J)$ improves the agreement so much.

The first thing we have to understand is why $E(j^2J)$ and $(j^2J\,|\,V_{12}\,|\,j^2J)$ are different. The fact that they are different means that our approximation is not good, and that if we are working in the pure shell-model scheme we are not allowed to neglect the non-diagonal elements of the energy matrix (2).

These non-diagonal elements have the form $(j^2J\,|\,V_{12}\,|\,j'j''J)$, and contribute to the energy in second approximation by an amount

$$\sum_{j'j''}\frac{(j^2J\,|\,V_{12}\,|\,j'j''J)^2}{2\varepsilon_j-\varepsilon_{j'}-\varepsilon_{j''}}\,, \tag{45}$$

which will be the difference (in second approximation) between $E(j^2J)$ and $(j^2J\,|\,V_{12}\,|\,j^2J)$.

Now it can be shown that the matrix elements which connect the configuration j^n with the configuration $j^{n-2}j'j''$ have the expression

$$\begin{aligned}(j^n\alpha J\,|\,V_{ik}\,|\,j^{n-2}\alpha_1J_1,\,j'j''J_2,\,J) &= \\ &= [\tfrac{1}{2}\,n(n-1)]^{\frac{1}{2}}(j^n\alpha J\,\{|\,j^{n-2}\alpha_1J_1,\,j^2J_2,\,J)(j^2J_2\,|\,J_{12}\,|\,j'j''J_2)\,,\end{aligned} \tag{46}$$

and therefore the second-order effects of these matrix elements will change the diagonal elements of (44) by the same amount by which they would be changed when we substitute in their expression $(j^2J\,|\,V_{12}\,|\,j^2J)$ with $E(j^2J)$.

This does not mean that this substitution takes into account all second order effects, because (46) holds only if both j' and j'' are different from j. This method does not account in the right measure for the second order perturbations produced by the configurations $j^{n-1}j'$, but we think that these effects are less important than the effects produced by the configurations $j^{n-2}j'^2$, and therefore conclude that the substitution of $(j^2J\,|\,V_1\,|\,j^2J)$ with $E(j^2J)$ takes into account the most important part of the second-order effects.

This conclusion agrees with the theory of Brueckner, according to which the substitution of the theoretical interaction with an « effective » interaction makes it possible to introduce into the first approximation the most important contributions of the higher approximations.

4. - The concept of seniority.

The methods developed in the preceding sections are sufficient in principle for calculating the coefficients of fractional parentage (cfp) and the energy matrix for any configuration j^n. But the calculations are in general very long and the results very complicated; we want therefore to look for methods which may simplify the calculations and the results.

The cfp are defined by eqs. (29) and (31) as eigenvectors corresponding to the eigenvalue 1 of the antisymmetrizator A. If this eigenvalue is not simple, the eigenvectors are not uniquely defined, and we may change the set of basic eigenvectors and the scheme of the energy matrix by a unitary transformation. It is our purpose to choose the scheme in such a way, that both the cfp and the energy matrix will be simplified as much as possible. This does not mean that the energy matrix will be diagonal in this scheme; but we shall see that there are good reasons for thinking that this scheme is not very far from the scheme in which the energy matrix is diagonal.

The method we use for building a particularly simple state of the configuration j^n, is to start from a state of the configuration j^v, to add to it $\frac{1}{2}(n-v)$ pairs of nucleons, each of which has resultant angular momentum equal to zero (« saturated pairs »), and to antisymmetrize the eigenfunction. If the original state of the configuration j^v did not contain saturated pairs, we shall say that the new state has a « seniority » v.

A state of seniority v has many properties which are similar to those of the original state of the configuration j^v, because a saturated pair has not only a vanishing angular momentum, but also vanishing multipole moments of odd order. Therefore all the multipole moments of odd order are equal in the original state and in the final state.

The multipole moments of even order do not vanish in a saturated pair, but they do not have a definite orientation and can take any orientation which is not forbidden by the Pauli principle. The number of allowed orientations is $j+\frac{1}{2}-v$, and it may therefore be shown that the expectation value of a multipole moment of even order for a state of seniority v may be calculated by multiplying the value for the original state of the configuration j^v by a « depolarization factor » $(j+\frac{1}{2}-n)/(j+\frac{1}{2}-v)$.

The number of saturated pairs may be measured by the operator

$$Q = \sum_{i<k} q_{ik} \,, \tag{47}$$

where q_{k} is a two-particle operator which vanishes if the angular momentum of the pair is different from zero, and has the value $2j+1$ if the pair is saturated:

$$(j^2 J \,|\, q_{12} \,|\, j^2 J) = (2j+1)\delta_{J0} \,. \tag{48}$$

For a state of seniority v the operator Q has the eigenvalue

$$Q(n, v) = \tfrac{1}{2}(n-v)(2j+3-n-v); \tag{49}$$

this value is smaller than $\frac{1}{2}(n-v)(2j+1)$, because the antisymmetrization reduces the weight of the saturated pairs.

In a scheme where Q is diagonal we shall substitute for the quantum number α the seniority number v and a further quantum number β, which will only distinguish, if necessary, between states with the same seniority and the same value of J. States of seniority v will have the same value of β as the state of j^v from which they originate. It follows that the coefficient of fractional grand-parentage $(j^{n-2}v_1\beta_1 J, j^2\, J_2 = 0, J]\} j^n v\beta J)$ will be different from zero only if $v_1 = v$ and $\beta_1 = \beta$, and substituting Q for V in (44), we get

$$(j^{n-2}v_1\beta_1 J, (j^2)_0, J]\} j^n v\beta J) = \sqrt{\frac{(n-v)(2j+3-n-v)}{n(n-1)(2j+1)}}\, \delta_{vv_1}\delta_{\beta\beta_1} \,. \tag{50}$$

If we express $\psi(j^n)$ as linear combination of $\psi(j^{n-1}j)$ with $\psi(j^{n-1})$ as linear combination of $\psi(j^{n-3}j^2)$, express on the other hand $\psi(j^n)$ as linear combination of $\psi(j^{n-2}j^2)$ with $\psi(j^{n-2})$ as linear combination of $\psi(j^{n-3}j)$, and compare the two expansions, we obtain

$$\begin{aligned}(j^{n-3}v'\beta'J', (j^2)_0, J']\} j^{n-1}v'\beta'J')(j^{n-1}v'\beta'J', j, J]\} j^n v\beta J) &= \\ = (j^{n-3}v'\beta'J', j, J]\} j^{n-2}v\beta J)(j^{n-2}v\beta J, (j^2)_0, J]\} j^n v\beta J) &\,,\end{aligned} \tag{51}$$

and owing to (50),

$$\begin{aligned}(j^{n-1}v'\beta'J', j, J]\} j^n v\beta J) &= \\ = \sqrt{\frac{(n-v)(2j+3-n-v)(n-2)}{(n-v'-1)(2j+4-n-v')n}}\,(j^{n-3}v'\beta'J', j, J]\} j^{n-2}v\beta J) &\,.\end{aligned} \tag{52}$$