SOCIETÀ ITALIANA DI FISICA

RENDICONTI
DELLA
SCUOLA INTERNAZIONALE DI FISICA
«ENRICO FERMI»

XV Corso

Spettroscopia Nucleare

ACADEMIC PRESS - NEW YORK AND LONDON

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XV Corso

a cura di G. Racah

Direttore del Corso

VARENNA SUL LAGO DI COMO

VILLA MONASTERO

20 GIUGNO - 9 LUGLIO 1960

Spettroscopia Nucleare

ACADEMIC PRESS • *NEW YORK AND LONDON*

ACADEMIC PRESS INC.
111 FIFTH AVENUE
NEW YORK 3, N. Y.

United Kingdom Edition
Published by
ACADEMIC PRESS INC. (LONDON) LTD.
BERKELEY SQUARE HOUSE, LONDON W. 1

Library of Congress Catalog Card Number: 62-13641

PRINTED IN ITALY

ITALIAN PHYSICAL SOCIETY

PROCEEDINGS

OF THE

INTERNATIONAL SCHOOL OF PHYSICS
« ENRICO FERMI »

XV Course

edited by G. Racah

Director of the Course

VARENNA ON LAKE COMO

VILLA MONASTERO

JUNE 20 - JULY 9 1960

Nuclear Spectroscopy

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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.

SOCIETÀ ITALIANA DI FISICA

SCUOLA INTERNAZIONALE DI FISICA «E. FERMI»

XV CORSO - VARENNA SUL LAGO DI COMO - VILLA MONASTERO - 20 Giugno - 9 Luglio 1960

Tipografia Compositori - Bologna - Italy

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LEZIONI

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

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

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

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

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

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

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

$$(12\,|\,j_a j_b J M) = \sum_{m_a m_b} (1\,|\,j_a m_a)(2\,|\,j_b m_b)(j_a m_a j_b m_b\,|\,j_a j_b J M)\,. \tag{11}$$

Permutation of the particle coordinates yields the eigenfunctions

$$(21\,|\,j_a j_b J M) = \sum_{m_a m_b} (2\,|\,j_a m_a)(1\,|\,j_b m_b)(j_a m_a j_b m_b\,|\,j_a j_b J M)\,, \tag{12}$$

and using the symmetry property (7) these eigenfunctions become

$$(-1)^{j_a+j_b-J} \sum_{m_a m_b} (2\,|\,j_a m_a)(1\,|\,j_b m_b)(j_b m_b j_a m_a\,|\,j_b j_a J M) = (-1)^{j_a+j_b-J}(12\,|\,j_b j_a J M)\,. \tag{13}$$

Therefore

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

In the particular case $j_a = j_b = j$ the eigenfunction on the right side of (14) coincides with (11), and therefore $(12\,|\,j^2 J M)$ 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 $(12\}j_a j_b J M)$, and write

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

or

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

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

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

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

The equation

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

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

$$(18) \qquad (123\}j_a j_b j_c J_{ab} JM) = \frac{1}{\sqrt{6}}[(123\,|\,j_a j_b j_c J_{ab} JM) - (213\,|\,j_a j_b j_c J_{ab} JM) +$$

$$+ (231\,|\,j_a j_b j_c J_{ab} JM) - (321\,|\,j_a j_b j_c J_{ab} JM) + (312\,|\,j_a j_b j_c J_{ab} JM) - (132\,|\,j_a j_b j_c J_{ab} JM)]\,.$$

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

$$(19) \qquad (12\}3\,|\,j^2 J_0,\, jJM) = \sum_{M_0 m} (12\}j^2 J_0 M_0)(3\,|\,jm)(J_0 M_0 jm\,|\,J_0 jJM) \qquad (J_0 \text{ even})\,,$$

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

$$(20) \qquad A(12\}3\,|\,j^2 J_0,\, jJM) =$$

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

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

$$(21a) \qquad (23\}1\,|\,j^2 J_0,\, jJM) =$$

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

and the third term is

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

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

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

where

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

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

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

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

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

from which we get that

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

Therefore the functions

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

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

$$(123\} j^3\alpha J M) = \sum_{J'} (12\}3\,|\,j^2J',\, jJ\,M)(j^2J',\, j,\, J\} j^3\alpha J)\,, \tag{28}$$

and the coefficients of this expansion satisfy the equation

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

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 $(12 \ldots r-1\}r\,|\,j^{r-1}\alpha_0 J_0,\, j,\, JM)$, which are antisymmetric only with respect to the first $r-1$ nucleons, and by taking those linear combinations of them,

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

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

$$\sum_{\alpha' J'} (\alpha_0 J_0\,|\,A(J)\,|\,\alpha' J')(j^{r-1}\alpha' J',\, j,\, J\} j^r\alpha J) = (j^{r-1}\alpha_0 J_0,\, j,\, J\} j^r\alpha J)\,, \tag{31}$$

where

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

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

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

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 $r_{12}^2 = r_1^2 + r_2^2 - 2r_1 r_2 \cos \omega_{12}$, 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

$$\begin{aligned} (n_a l_a j_a n_b l_b j_b J M \,|\, V(r_{12}) \,|\, n_c l_c j_c n_d l_d j_d J M) = \\ = \sum_k R^k(n_a l_a n_b l_b, n_c l_c n_d l_d) (l_a j_a l_b j_b J M \,|\, P_k(\cos \omega_{12}) \,|\, l_c j_c l_d j_d J M) , \end{aligned} \tag{36}$$

where the R^k are the generalized Slater integrals

$$R^k(n_a l_a n_b l_b, n_c l_c n_d l_d) = \iint R_{n_a l_a}(r_1) R_{n_b l_b}(r_2) v_k(r_1, r_2) R_{n_c l_c}(r_1) R_{n_d l_d}(r_2) \, dr_1 \, dr_2 . \tag{37}$$