# ON THE PHASE FACTORS FOR TRANSITION FROM "PARTICLE" TO "HOLE" STATES IN THE NUCLEAR-SHELL THEORY

V. V. BALASHOV

Institute of Nuclear Physics, Moscow State University

Submitted to JETP editor September 11, 1958

J. Exptl. Theoret. Phys. (U.S.S.R.) 36, 1387-1392 (May, 1959)

The method of second quantization, applied in reference 1 to the calculation of matrix elements for F and G operators of shell theory, is used to obtain a relation between fractional parentage coefficients of the beginning and the end of the shell. The change of the phase factors in the transition from "particle" to "hole" states is investigated. Selection rules for electromagnetic transitions in nuclei due to the symplectic group are found for the case of jj-coupling.

1. In a paper by Tumanov, Shirokov and the author[1] a method based on second quantization was developed to calculate matrix elements of a single particle (F) and a two particle (G) operator for the general case of mixed particle or hole configurations. In the present work we shall obtain some formulae of matrix elements of F operators for hole configurations which have not been given in reference 1. We shall utilize these to obtain a connection between the fractional parentage coefficients for the beginning and the end of a shell, and to obtain new selection rules for electromagnetic transitions in nuclei.

The wave function of a closed shell nucleon state forms a representation of the group of rotations in the usual and the isotopic spin space with $J = 0$ and $T = 0$ and of the symplectic group with $(\sigma) = (00)$. We therefore can consider this state to form the "vacuum" of particles and a state in which one particle is missing from the closed shell as a "hole" in the "vacuum" state. The transition from the nucleon annihilation operator $b(j, m, \tau)$ for the state $j, m, \tau$ to the creation operator for the corresponding hole state which has the proper exchange symmetries is given by

$$b(j, m, \tau) = (-1)^{j+m}(-1)^{1/2+\tau} C^{+}(j, -m, -\tau), \quad (1)$$

where j is the angular momentum of a nucleon m is its projection and $\tau$ is the projection of the isotopic spin.

Utilizing Eq. (36) of reference 1 for the F operator and for the transition of the particle wave function $|j^{n_0-n}(\sigma)JT\rangle$ to the hole wave function $|j^{-n}(\sigma)JT\rangle$ (where $n_0 = 2(2j+1)$ is the number of particles in the closed shell) we express the matrix elements in terms of the reduced matrix elements $\langle j_1 \| f_{k\kappa} \| j_2 \rangle$ after some not too complicated transformations involving Clebsch-Gordan coefficients:

$$\begin{aligned}\langle j^{-n}(\sigma)JT \,|\, f_{k\varkappa} \,|\, j^{-n}(\sigma')J'T'\rangle &= -n(-1)^{x}(-1)^{x'}(-1)^{k}(-1)^{\varkappa} \\ &\times \sum \langle j^{n}(\sigma)JT \,|\, j^{n-1}(\tilde{\sigma})\tilde{J}\tilde{T}\rangle \langle j^{n}(\sigma')J'T' \,|\, j^{n-1}(\tilde{\sigma})\tilde{J}\tilde{T}\rangle \\ &\times U(\tilde{J}jJ'k : Jj)\, U(\tilde{T}{}^1/_2 T'\varkappa : T{}^1/_2)\langle j \| f_{k\varkappa} \| j\rangle. \quad (2)\end{aligned}$$

Here k and $\kappa$ are the degrees of the operator F in space and isotopic spin space respectively, $U(j_1 j_2 J j_3 : J_{12} J_{23})$ are Racah coefficients,[2] $(-1)^{X}$ and $(-1)^{X'}$ are phase factors due to the particle $\to$ hole transition, and $\langle j^{n}(\sigma)JT | j^{n-1}(\sigma')J'T'\rangle$ are the fractional parentage coefficients.[3]

In a similar fashion we obtain an expression for mixed hole configurations employing the transformation Eq. (26) of reference 1:

$$\begin{aligned}\langle j_1^{-(n+1)}J_1T_1,\ j_2 : JT \,|\, f_{k\varkappa} \,|\, j_1^{-n}J'T'\rangle &= -(-1)^{n}\sqrt{n+1}\,(-1)^{k-j_1-j_2}(-1)^{\varkappa-1}(-1)^{x}(-1)^{x'} \\ &\times \left[\frac{2(2j_2+1)}{(2k+1)(2\varkappa+1)}\right]^{1/2} \langle j_1^{n+1}J_1T_1 \,|\, j_1^{n}J'T'\rangle\, U(J'j_1Jj_2 : J_1k) \\ &\times U(T'{}^1/_2 T{}^1/_2 : T_1\varkappa)\langle j_1 \| f_{k\varkappa} \| j_2\rangle. \quad (3)\end{aligned}$$

2. The matrix element (3), calculated here through the use of the hole concept, can also be obtained in a different fashion, namely by using fractional parentage coefficients for configurations filling the shell by more than one half:

$$\begin{aligned}\langle j_1^{n_0-(n+1)}J_1T_1,\ j_2 : JT \,|\, f_{k\varkappa} \,|\, j_1^{n_0-n}J'T'\rangle &= \sqrt{n_0-n}\,(-1)^{n_0-n-1}\langle j_1^{n_0-n}J'T' \,|\, j_1^{n_0-n-1}J_1T_1\rangle \\ &\times U(J_1j_1Jk : J'j_2)\, U(T_1{}^1/_2 T\,k : T'{}^1/_2)\langle j_1 \| f_{k\varkappa} \| j_2\rangle. \quad (4)\end{aligned}$$

Utilizing the known property of the Racah coefficients

$$U(j_1j_2Jj_3 : J_{12}J_{23})$$
$$= (-1)^{J_{12}+J_{23}-j_1-j_3}\left[\frac{(2J_{12}+1)(2J_{23}+1)}{(2j_1+1)(2j_3+1)}\right]^{1/2} U(J_{12}j_2JJ_{23} : j_1j_3),$$

we obtain by equating (3) and (4) a relation between the fractional parentage coefficients for the beginning and the end of the shell:

$$\langle j^{n_0-n}(\sigma)JT \mid j^{n_0-(n+1)}(\sigma')J'T'\rangle$$
$$= (-1)^{x}(-1)^{x'}(-1)^{J-J'-j}(-1)^{T-T'-1/2}$$
$$\times\left[\frac{(n+1)(2J'+1)(2T'+1)}{(n_0-n)(2J+1)(2T+1)}\right]^{1/2}$$
$$\times\langle j^{n+1}(\sigma')J'T' \mid j^{n}(\sigma)JT\rangle. \qquad (5)$$

3. Setting the phase factors $(-1)^X$ and $(-1)^{X'}$ equal to unity in (5) we arrive at the known result connecting the fractional parentage coefficients for $n > n_0/2$ with those for $n < n_0/2$, derived by Rosenzweig[4] for the case of L–S coupling and extended to j–j coupling by Smirnov.[5] However, such an arbitrary choice of the phases is possible only if we consider the beginning and the end of the shell separately. In going through the middle of the shell it does not work. The formulae obtained in references 4 and 5 do not allow to join the results obtained for $n = n_0/2$ with holes or with particles, and they lead to wrong results when trying to compute double fractional parentage coefficients (for splitting off two particles).

Let us consider as an example the coefficients $\langle(3/2)^5(21)\,\tfrac{1}{2}\tfrac{1}{2}\mid(3/2)^4(\sigma)\,JT\rangle$. Disregarding the phase factors in (5) we obtain

$$\langle(3/2)^5(21)\,1/2\,1/2\mid(3/2)^4(11)\,20\rangle = -1/2\sqrt{5},$$
$$\langle(3/2)^5(21)\,1/2\,1/2\mid(3/2)^4(22)\,20\rangle = -\sqrt{7}/2\sqrt{5},$$
$$\langle(3/2)^5(21)\,1/2\,1/2\mid(3/2)^4(20)\,11\rangle = -3/2\sqrt{5},$$
$$\langle(3/2)^5(21)\,1/2\,1/2\mid(3/2)^4(11)\,21\rangle = \sqrt{3}/2\sqrt{5}. \qquad (6)$$

The fractional parentage coefficients must obey the following orthogonality relations:

$$\sum\langle j^{n}(\sigma)JT\mid j^{n-1}(\sigma')J'T'\rangle\langle j^{n-1}(\sigma')J'T'\mid j^{n-2}(\sigma'')J''T''\rangle$$
$$\times U(J''jJj : J'J_0)\,U(T''\,1/2\,T\,1/2 : T'T_0) = 0, \qquad (7)$$

if $J_0 + T_0$ is even. One can easily see that this relation is not fulfilled by the coefficients (6). A direct computation of these coefficients from solving a system of linear equations (the Racah method) yields

$$\langle(3/2)^5(21)\,1/2\,1/2\mid(3/2)^4(11)\,20\rangle = 1/2\sqrt{5},$$
$$\langle(3/2)^5(21)\,1/2\,1/2\mid(3/2)^4(22)\,20\rangle = -\sqrt{7}/2\sqrt{5},$$
$$\langle(3/2)^5(21)\,1/2\,1/2\mid(3/2)^4(20)\,11\rangle = 3/2\sqrt{5},$$
$$\langle(3/2)^5(21)\,1/2\,1/2\mid(3/2)^4(11)\,21\rangle = \sqrt{3}/2\sqrt{5}. \qquad (8)$$

This example illustrates an important circumstance. The first two coefficients of which one changes sign while the other does not correspond to a transition into states with the same J and T but with different $(\sigma)$. This indicates that the change in the phase in the transition from $n > n_0/2$ to $n < n_0/2$ is connected with the character of the state with respect to the symplectic group. These characteristics were usually disregarded when considering the connection between particle and hole states. They also are not evident in (1). The introduction of additional phase factors into (1) is connected with the peculiarities in the vector addition for hole configurations and has nothing to do with the change of the symplectic character in the transition from particle to hole states. These have to be accounted for separately.

The question on the phase changes in the transition from particle to hole states in the case of LS-coupling has been fully treated by Racah in his original papers on the theory of atomic configurations.[2,6] Considering consecutively the possible transitions in seniority: $v \to v+1$ and $v \to v-1$ he obtains a simple expression connecting the phase change of the configuration $|l^n vSL\rangle$ with n and v. In connection with nuclei this question, also in LS-coupling, has been investigated by Jahn.[7] The question of the phase change has not been treated for jj-coupling.

According to the group-theoretical classification of states in the scheme of jj-coupling,[8] the wave function for a nucleon state forms a representation of the permutation group, the symplectic group, and the group of three dimensional rotations and consequently can be characterized by the quantum numbers T, $(\sigma)$ (or, equivalently by s – the seniority and t – the reduced isotopic spin) and J. The problem consists in connecting the phase change in the particle—hole transition with these quantum numbers.

This problem can be solved in the same way as Racah proceeded in the case of atoms.[6] By utilizing the Kasimir operator,[3,8,9] the eigenvalues of which denumerate the representations of the symplectic group, one thus has to obtain a recursion relation for the fractional parentage coefficients

$$\langle j^{n}(\sigma)JT\mid j^{n-1}(\sigma')J'T'\rangle \text{ and } \langle j^{n-2}(\sigma)JT\mid j^{n-3}(\sigma')J'T'\rangle.$$

This way the transition from particles to holes will not occur at $n = n_0/2$ but at a smaller n. There the choice of the phases is unimportant and one can utilize (5) with an arbitrary choice of the phases. One can easily understand that such a procedure will lead to phases which in the general case will depend linearly on the quantum numbers of the state. The practical difficulty associated with such an approach is due to the fact that here in contrast to the atomic case the seniority is characterized by two instead of one number. Consequently the number of the possible transitions is much larger. They have to be considered in order to find the dependence of the phase on these quantum numbers.

There exists another simpler procedure for solving this problem. It is based on the fact that the condition of the linear dependence of the phase on s and t allows to construct uniquely general expressions for the phase in terms of these quantum numbers. Since the phase change which is connected with the symplectic group does not depend on J we have

$$(-1)^x = (-1)^{\alpha(n-s)/2+\beta(T-t)}. \qquad (9)$$

Here $\alpha$ and $\beta$ are certain still undetermined integers (obviously, either zero or unity). We remark that in the atomic case the expression $(-1)^{(n-v)/2}$ is a generalization of Racah's Eq. (65) of reference 6 for the phase. We shall find the constants $\alpha$ and $\beta$ if we succeed to determine the phases independently of (5) for some arbitrary "basis" set of states. We utilize for this purpose the fact that the orthogonality relations (7) are true for arbitrary n and thus the computation of the fractional parentage coefficients from a set of linear equations (the orthogonality relations) does not only yield their values but also their phases. The "basis" set of states used to obtain $\alpha$ and $\beta$ can be arbitrary. It just has to be sufficiently large, i.e., it must contain a sufficiently large number of independent equations. This condition is, for example, fulfilled by the above considered set of states $|(3/2)^4(\sigma)\, JT\rangle$, which is connected by the fractional parentage coefficients (8) with the state $|(3/2)^5\,(21)\tfrac{1}{2}\tfrac{1}{2}\rangle$. Comparing (6) and (8) we find $\alpha = 0$, $\beta = 1$. Thus

$$(-1)^x = (-1)^{T-t}. \qquad (10)$$

The constants $\alpha$ and $\beta$ of (9) do not depend on j. Therefore the relation (10) which has been obtained for j = 3/2 has general validity for arbitrary j.

Taking (10) into account, Eq. (5) assumes the final form:

$$\langle j^{n_0-n}(\sigma)\, JT\,|\, j^{n_0-(n+1)}(\sigma')\, J'T'\rangle = (-1)^{J-J'-j}(-1)^{t-t'-1/2}\left[\frac{(n+1)(2J'+1)(2T'+1)}{(n_0-n)(2J+1)(2T+1)}\right]^{1/2} \times \langle j^{n+1}(\sigma')\, J'T'j\,|\, j^n(\sigma)JT)\rangle. \qquad (11)$$

In the Appendix we give tables of fractional parentage coefficients which supplement the well known tables of Edmunds and Flowers.[3]

**4.** We shall now apply the obtained results to the calculation of the probability of electromagnetic transitions in nuclei which consist of half filled shells: $n = n_0/2 = 2j+1$. The matrix element $M_{12}(l, \kappa)$ for the transition of multipolarity $l$ and isotopic multiplicity $\kappa$ is given by the equation

$$M_{12}(l,\varkappa) = \langle j^n(\sigma)\, JT\,|\, Q(l,\varkappa)\,|\, j^n(\sigma')\, J'T'\rangle = n\Sigma\langle j^n(\sigma)\, JT\,|\, j^{n-1}(\tilde\sigma)\,\tilde J\tilde T\rangle\langle j^n(\sigma')\, J'T'\,|\, j^{n-1}(\tilde\sigma)\,\tilde J\tilde T\rangle \times U(\tilde J jJ'l : Jj)\, U(\tilde T\, {}^1\!/_2\, T'\varkappa : T\, {}^1\!/_2)\langle j\,\|\, Q(l,\varkappa)\,\|\, j\rangle. \qquad (12)$$

The same element can be written down by means of (2). This way we obtain

$$M_{12}(l,\varkappa) = -(-1)^l(-1)^\varkappa \times (-1)^{T_1-t_1}(-1)^{T_2-t_2} M_{12}(l,\varkappa). \qquad (13)$$

Equation (13) expresses a selection rule due to the symplectic group for electromagnetic transitions in the case of jj-coupling. It is not contained in the selection rules with respect to the seniority s which have been given by Neudachin.[10] In particular, if the isotopic spin $T_2$ and the reduced isotopic spin $t_2$ in the final state equal zero (e.g., in the ground state of the nucleus) then $t_1$ and $l$ are connected by the relation

$$t_1 + l = \text{odd number} \qquad (14)$$

In this connection, for example, in $Be^8$ the E2 transition from the level 20 (22) to the ground state is forbidden while the M1 transition from the level 20 (11) is allowed. Similarly the M1 transitions from the levels 11 (20) and 31 (20) to the level 20 (11) are forbidden as well as E2 transitions from these levels to the level 20 (22). These transitions are allowed by the selection rules of reference 10. Naturally, the rigorous forbiddeness of the given examples will be spoiled by the admixture of the $p_{\frac{1}{2}}$ configuration. However, the indicated regularities can be utilized to identify the levels of this nuclide. Of much greater interest is the application of this selection rule to heavier nuclei where jj-coupling obtains. Selection rules, analogous to (13), can be also obtained for LS-coupling.

**5.** In conclusion we give the formula for the particle to hole transition of double fractional parentage coefficients which follows immediately from Eqs. (32) and (48) of reference 1:

$$\langle j^{n_0-n}(\sigma)\, JT\,|\, j^{n_0-(n+2)}(\sigma')\, J'T',\; j^2J_0T_0\rangle = (-1)^{J-J'}(-1)^{t-t'} \times\left[\frac{(n+2)(n+1)}{(n_0-n)(n_0-n-1)}\,\frac{(2J'+1)(2T'+1)}{(2J+1)(2T+1)}\right]^{1/2} \times\langle j^{n+2}(\sigma')\, J'T'\,|\, j^n(\sigma)\, JT,\; j^2J_0T_0\rangle.$$

The author thanks V. G. Neudachin for a useful discussion.

## APPENDIX

Fractional parentage coefficients $\langle (3/2)^5 JT(\sigma) | (3/2)^4 (\sigma') J'T' \rangle$

| $J'T'(\sigma')$ | $JT(\sigma)$ | | | | |
|---|---|---|---|---|---|
| | $\frac{1}{2}\,\frac{1}{2}$ (21) | $\frac{3}{2}\,\frac{1}{2}$ (10) | $\frac{5}{2}\,\frac{1}{2}$ (21) | $\frac{7}{2}\,\frac{1}{2}$ (21) | $\frac{3}{2}\,\frac{3}{2}$ (10) |
| 00 (00) | — | $1/\sqrt{10}$ | — | — | — |
| 20 (11) | $1/2\sqrt{5}$ | $-\sqrt{3/10}$ | $-1/2\sqrt{5}$ | $-1/2\sqrt{5}$ | — |
| 20 (22) | $-\sqrt{7}/2\sqrt{5}$ | — | $-\sqrt{5}/2\sqrt{7}$ | $1/\sqrt{35}$ | — |
| 40 (22) | — | — | $-\sqrt{6/35}$ | $-3/2\sqrt{7}$ | — |
| 11 (20) | $3/2\sqrt{5}$ | $-\sqrt{3}/5\sqrt{2}$ | $\sqrt{21}/10$ | — | $-\sqrt{3}/2\sqrt{5}$ |
| 21 (11) | $\sqrt{3}/2\sqrt{5}$ | $\sqrt{2/5}$ | $-\sqrt{3}/2\sqrt{5}$ | $-\sqrt{3}/2\sqrt{5}$ | $-1/2$ |
| 31 (20) | — | $-\sqrt{7}/5\sqrt{2}$ | $-\sqrt{6}/5$ | $3/2\sqrt{5}$ | $-\sqrt{7}/2\sqrt{5}$ |
| 02 (00) | — | — | — | — | $1/2$ |

Fractional parentage coefficients $\langle (3/2)^6 JT(\sigma) | (3/2)^5 J'T'(\sigma') \rangle$

| $J'T'(\sigma')$ | $JT(\sigma)$ | | | |
|---|---|---|---|---|
| | 01 (00) | 10 (20) | 21 (11) | 30 (20) |
| $\frac{1}{2}\,\frac{1}{2}$ (21) | — | $1/\sqrt{3}$ | $1/\sqrt{15}$ | — |
| $\frac{3}{2}\,\frac{1}{2}$ (10) | $-\sqrt{5}/3$ | $-1/\sqrt{5}$ | $1/3\sqrt{5}$ | $1/\sqrt{5}$ |
| $\frac{5}{2}\,\frac{1}{2}$ (21) | — | $\sqrt{7/15}$ | $-1/\sqrt{5}$ | $2\sqrt{2}/\sqrt{35}$ |
| $\frac{7}{2}\,\frac{1}{2}$ (21) | — | — | $2/\sqrt{15}$ | $2/\sqrt{7}$ |
| $\frac{3}{2}\,\frac{3}{2}$ (10) | $2/3$ | — | $2/3$ | — |

[1]Balashov, Tumanov and Shirokov, Ядерные реакции при малых и спедних энергиях. Труды Всесоюзной конференции, ноябрь, 1957 г. (Nuclear Reactions at Small and Medium Energies). Proceedings of the All-Union Conference, Nov. 1957, U.S.S.R., Acad. of Sci. Press (1958).

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

[3]A. R. Edmonds and B. H. Flowers, Proc. Roy. Soc. A214, 515 (1952).

[4]N. Rosenzweig, Phys. Rev. **88**, 580 (1952).

[5]Iu. F. Smirnov, Diploma thesis, Moscow State University (1957) (unpublished).

[6]G. Racah, Phys. Rev. **63**, 367 (1943)

[7]H. A. Jahn and H. Van Wieringen, Proc. Roy. Soc. **A209**, 502 (1951).

[8]B. H. Flowers, Proc. Roy. Soc. **A212**, 248 (1952).

[9]G. Racah, Group Theory and Spectroscopy, (Lecture Notes) Inst. Adv. Study, Princeton (1951).

[10]V. G. Neudachin, J. Exptl. Theoret. Phys. (U.S.S.R.) **31**, 891 (1956), Soviet Phys. JETP **4**, 751, (1957).

Translated by M. Danos
275