Alternative Mathematical Technique to Determine LS Spectral Terms

Renjun Xu[1,2,*] and Zhenwen Dai[2,3,†]

[1]National Laboratory of Super Hard Materials,

Jilin University, Changchun 130012, P.R. China

[2]College of Physics, Jilin University, Changchun 130023, P. R. China

[3]Key Lab of Coherent Light, Atomic and Molecular Spectroscopy,

Ministry of Education, Jilin University, Changchun 130023, P.R. China

Abstract

We presented an alternative computational method for determining the permitted LS spectral terms arising from l^N electronic configurations. This method makes the direct calculation of LS terms possible. Using only basic algebra, we derived our theory from LS-coupling scheme and Pauli exclusion principle. As an application, we have performed the most complete set of calculations to date of the spectral terms arising from l^N electronic configurations, and the representative results were shown.[1] As another application on deducing LS-coupling rules, for two equivalent electrons, we deduced the famous Even Rule; for three equivalent electrons, we derived a new simple rule.

PACS numbers: 31.15.-p, 31.10.+z, 71.70.Ej, 02.70.-c

---

[1] The table of LS terms for $l^N(l = 0$–$5)$ configurations is too long and over two pages, so we only present part of the result in this article.

*E-mail: xu5n@yahoo.com

†E-mail: jzk@mail.jlu.edu.cn

I.   INTRODUCTION

In the atomic and nuclear shell model, a basic but often laborious and complicated problem is to calculate the spectral terms arising from many-particle configurations. For a N-particle occupied subshell l^N, currently we often use computational methods based on the unitary-group representation theory, which have been developed by Gelfand et al. [1], M. Moshinsky et al. [2], Biedenharn et al. [3], Judd [4], Louck et al. [5], Drake et al. [6], Harter et al. [7], Paldus [8], Braunschweig et al. [10], Kent et al. [11] and others, extending thus the classical works of Weyl [12], Racah [13], S. Meshkov [14], Cartan, Casimir, Killing, and others. For efforts of all these works, can we have the current calculation method much more simplified and less steps needed than ever before. However, when many electrons with higher orbital angular momentum are involved in one subshell, the calculation process using this theoretical method still is a challenging work. The current feasible methods usually take several steps of simplification, such as firstly using Branching Rules for reduction [10], and then using LL-coupling scheme. Nevertheless, we still have to work hard to calculate a big table of the LS terms corresponding to Young Patterns of one column (the situation is similar to use Gelfand basis set [7, 8, 9]), and many LL-couplings. Often this is a difficult and complicated job.

In this paper, we present an alternative mathematical technique for direct determination of spectral terms for l^N configurations. The new theory consists of a main formula [equation (1)] and four complete sub-formulas [equations (2)-(5)], all of which are common algebra expressions. The basis of this method does not require any knowledge of group theory or other senior mathematics.

The organization of this paper is as follows: the five basic formulas and some notations are introduced in Section II (the derivations of those formulas are presented in Appendix). The specific calculation procedure is shown in Section III. In Section VI, as some applications using this alternative theory, we presented permitted spectral terms for several l^N configurations; then deduced naturally the well-known Even Rule for two electrons; and for three electrons, we derived a new compact rule. Finally, conclusions are drawn in Section V.

II. THEORETICAL OUTLINE AND NOTATIONS

A. Notations

In the following, we denote by $X(N, l, S', L)$ the number of spectral terms with total orbital angular quantum number L and total spin quantum number $S'/2$ arising from l^N electronic configurations. (To calculate and express more concisely, we doubled the total spin quantum number S and the spin magnetic quantum number M_S here, which are correspondingly denoted by S' and M'_S. Hence, all discussions in the following are based on integers.) When the function $X(N, l, S', L) = 0$, it means that there is no spectral terms with total orbital angular quantum number L and spin quantum number $S'/2$. We denote by $A(N, l, l_b, M'_S, M_L)$ the number of LS terms having allowable orbital magnetic quantum number M_L and spin magnetic quantum number $M'_S/2$, arising from l^N electronic configurations. l_b is defined as the largest allowable orbital magnetic quantum number $(m_{l_i})_{\max}$ in one class. Its initial value equals l according to equation (1).

B. The Complete Basic Formulas

The main formula to calculate the number of LS terms in l^N electronic configurations is given below,

$$X(N, l, S', L) = A(N, l, l, S', L) - A(N, l, l, S', L+1)$$
$$+ A(N, l, l, S'+2, L+1) - A(N, l, l, S'+2, L), \tag{1}$$

where the value of function $\mathbf{A}$ is based on the following four sub-formulas

Case 1 : $M'_S = 1$, $|M_L| \le l$, and $N = 1$

$$A(1, l, l_b, 1, M_L) = 1 \tag{2}$$

Case 2 :
$$\{M'_S\} = \{2 - N, 4 - N, \ldots, N - 2\},$$
$$|M_L| \le f(\tfrac{N-M'_S}{2} - 1) + f(\tfrac{N+M'_S}{2} - 1), \text{ and } 1 < N \le 2l + 1$$

$$A(N, l, l, M'_S, M_L) = \sum_{M_{L_-} = \left\{-f(\frac{N-M'_S}{2}-1),\, M_L-f(\frac{N+M'_S}{2}-1)\right\}_{\max}}^{\left\{f(\frac{N-M'_S}{2}-1),\, M_L+f(\frac{N+M'_S}{2}-1)\right\}_{\min}} \left\{ A\left(\tfrac{N-M'_S}{2}, l, l, \tfrac{N-M'_S}{2}, M_{L_-}\right) \right.$$
$$\left. \times\, A\left(\tfrac{N+M'_S}{2}, l, l, \tfrac{N+M'_S}{2}, M_L - M_{L_-}\right) \right\} \tag{3}$$

Case 3 : $M'_S = N$, $|M_L| \le f(N - 1)$, and $1 < N \le 2l + 1$

$$A(N, l, l_b, N, M_L) = \sum_{M_{L_I} = \lfloor \frac{M_L - 1}{N} + \frac{N+1}{2} \rfloor}^{\{l_b,\, M_L + f(N-2)\}_{\min}} A(N - 1, l, M_{L_I} - 1, N - 1, M_L - M_{L_I}) \tag{4}$$

Case 4 : other cases just do not exist, therefore

$$A(N, l, l_b, M'_S, M_L) = 0 \tag{5}$$

where the floor function $\lfloor x \rfloor$ presented in this paper denotes the greatest integer not exceeding x, and

$$f(n) = \begin{cases} \sum\limits_{m=0}^{n} (l - m) & for\ n \ge 0 \\ 0 & for\ n < 0 \end{cases}$$

The derivations of equations (1)-(4) are presented in detail in Appendix.

III. THE SPECIFIC PROCEDURE

A concrete procedure to determine the LS spectral terms arising from l^N electronic configurations is given in Figure 1. For l^N electronic configurations, if N is larger than $(2l + 1)$ and less than $(4l + 2)$, it is equivalent to the case of $(4l + 2 - N)$ electrons; Else if N is not larger than $2l + 1$, the total spin quantum number S could be $\{\frac{N}{2} - \lfloor \frac{N}{2} \rfloor, \frac{N}{2} + 1 - \lfloor \frac{N}{2} \rfloor, \ldots, \frac{N}{2}\}$ [equations (C22, D1)], and the total orbital angular quantum number L could be $\{0, 1, \ldots, f(\frac{N-M'_S}{2} - 1) + f(\frac{N+M'_S}{2} - 1)\}$ [equation (C17)]. The number of LS terms with total orbital angular quantum number L and total spin quantum number S ($S = S'/2$) is calculated by function $X(N, l, S', L)$. Based on equation (1), then the main task is to calculate the function $A(N, l, l_b, M'_S, M_L)$. Due to the value of three
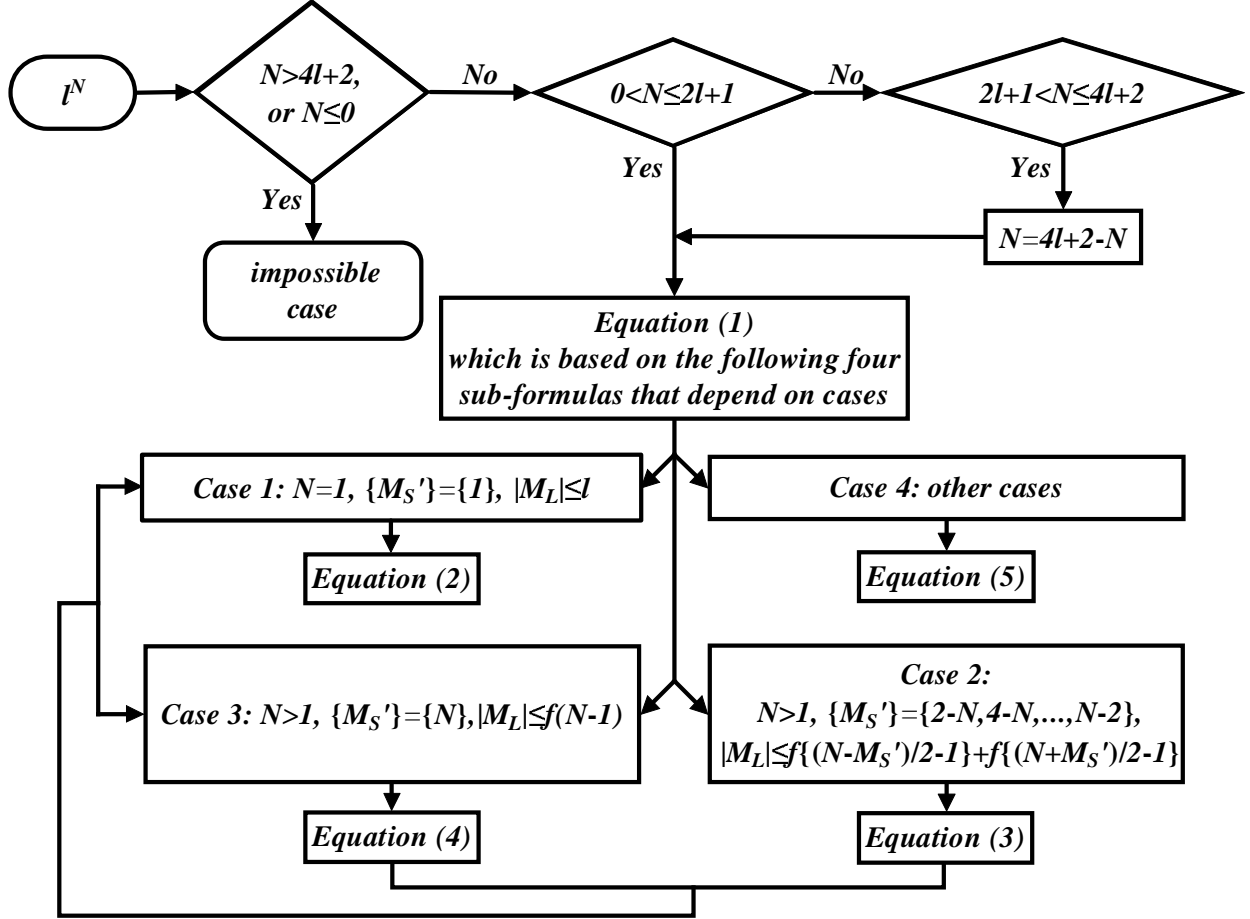
FIG. 1: Specific procedure to determine LS terms arising from l^N.

parameters N, M_S', and M_L in function **A**, there are four cases. If it is in the condition of case 2 or case 3, we can calculate the function **A** based on the equation (3) or equation (4), both of which could come down to case 1 or case 3. Finally, we will get the eigenvalue of function **X**. If the function **X** vanishes, it means that there is no corresponding LS terms.

IV. EXAMPLES AND APPLICATIONS

A. Permitted LS terms of l^N subshell

Based on the flow chart shown in Figure 1, we have written a computer program in C language. For the length limit of this article, we only presented in Table I the LS terms for g^9 and h^{11} electronic configurations. (The terms for s^N, p^N, d^N, and f^N can be found in Robert D. Cowan's textbook [15, p. 110].) As far as we know, LS spectral terms of g^N and

h^N given here are reported for the first time in literature.

The notation of the spectral terms given below is proposed by Russell [16] and Saunders [17] and now has been widely used.

$$L = 0 \quad 1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 6 \quad 7 \quad 8 \quad 9 \quad 10 \quad 11 \quad 12$$
$$\quad\quad S \quad P \quad D \quad F \quad G \quad H \quad I \quad K \quad L \quad M \quad N \quad O \quad Q$$
$$L = 13 \quad 14 \quad 15 \quad 16 \quad 17 \quad 18 \quad 19 \quad 20 \quad 21 \quad 22 \quad 23 \quad \cdots$$
$$\quad\quad R \quad T \quad U \quad V \quad W \quad X \quad Y \quad Z \quad 21 \quad 22 \quad 23 \quad \cdots$$

When the orbital quantum number L is higher than 20, it is denoted by its value. Owing to the length of the table, a compact format [18] of terms is given here: $^{A}(L_{k_1} L'_{k_2} \ldots)$, in which the superscript A indicates the multiplicity of all terms included in the parentheses, and the subscripts k_1, k_2 indicate the number of terms, for example $^2G_6$ means that there are six ^2G terms.

TABLE I: Permitted LS terms for selected l^N configurations.

Configurations	LS spectral terms
g^9	$^2(S_8\ P_{19}\ D_{35}\ F_{40}\ G_{52}\ H_{54}\ I_{56}\ K_{53}\ L_{53}\ M_{44}\ N_{40}\ O_{32}\ Q_{26}\ R_{19}\ T_{15}\ U_9\ V_7\ W_4\ X_2\ YZ)$
	$^4(S_6\ P_{16}\ D_{24}\ F_{34}\ G_{38}\ H_{40}\ I_{42}\ K_{39}\ L_{35}\ M_{32}\ N_{26}\ O_{20}\ Q_{16}\ R_{11}\ T_7\ U_5\ V_3\ W\ X)$
	$^6(S_3P_3D_9F_8G_{12}H_{10}I_{12}K_9L_9M_6N_6O_3Q_3RT)$ $^8(PDFGHIKL)$ $^{10}(S)$
h^{11}	$^2(S_{36}\ P_{107}\ D_{173}\ F_{233}\ G_{283}\ H_{325}\ I_{353}\ K_{370}\ L_{376}\ M_{371}\ N_{357}\ O_{335}\ Q_{307}\ R_{275}\ T_{241}\ U_{207}\ V_{173}$ $W_{142}\ X_{114}\ Y_{88}\ Z_{68}\ 21_{50}\ 22_{36}\ 23_{25}\ 24_{17}\ 25_{11}\ 26_7\ 27_4\ 28_2\ 29\ 30)$ $^4(S_{37}\ P_{89}\ D_{157}\ F_{199}$ $G_{253}\ H_{277}\ I_{309}\ K_{313}\ L_{323}\ M_{308}\ N_{300}\ O_{271}\ Q_{251}\ R_{216}\ T_{190}\ U_{155}\ V_{131}\ W_{101}\ X_{81}\ Y_{59}\ Z_{45}$ $21_{30}\ 22_{22}\ 23_{13}\ 24_9\ 25_5\ 26_3\ 27\ 28)$ $^6(S_{12}\ P_{35}\ D_{55}\ F_{76}\ G_{90}\ H_{101}\ I_{109}\ K_{111}\ L_{109}\ M_{105}$ $N_{97}\ O_{87}\ Q_{77}\ R_{65}\ T_{53}\ U_{43}\ V_{33}\ W_{24}\ X_{18}\ Y_{12}\ Z_8\ 21_5\ 22_3\ 23\ 24)$ $^8(S_4\ P_4\ D_{12}\ F_{11}\ G_{17}\ H_{15}$ $I_{19}\ K_{16}\ L_{18}\ M_{14}\ N_{14}\ O_{10}\ Q_{10}\ R_6\ T_6\ U_3\ V_3\ W\ X)$ $^{10}(PDFGHIKLMN)$ ^{12}S

B. Derivation of the Even Rule for two equivalent electrons

If only two equivalent electrons are involved, there is an "Even Rule" [19] which states

> For two equivalent electrons the only states that are allowed are those for which the sum $(L + S)$ is even.

This rule can be deduced from our formulas as below. Based on equations (3) and (2), when $0 \leq M_L \leq 2l$, we have

$$A(2, l, l, 0, M_L) = \sum_{M_{L_-} = \{-l, \, M_L - l\}_{\max}}^{\{l, \, M_L + l\}_{\min}} 1 = 2l - M_L + 1. \tag{6}$$

Based on equations (4) and (2), when $0 \leq M_L \leq 2l - 1$, we have

$$A(2, l, l_b, 2, M_L) = \sum_{M_{L_I} = \lfloor \frac{M_L}{2} + 1 \rfloor}^{\{l_b, \, M_L + l\}_{\min}} 1 \tag{7}$$

$$= l_b - \lfloor \frac{M_L}{2} \rfloor. \tag{8}$$

Hence, based on our main formula [equation (1)], we have

$$X(2, l, S', L) = \begin{cases} \lfloor \frac{L}{2} \rfloor - \lfloor \frac{L-1}{2} \rfloor & \text{when } S' = 0 \\ \lfloor \frac{L+1}{2} \rfloor - \lfloor \frac{L}{2} \rfloor & \text{when } S' = 2 \end{cases}$$

$$= \lfloor \frac{L+S}{2} \rfloor - \lfloor \frac{L+S-1}{2} \rfloor. \tag{9}$$

Therefore, only when $(L + S)$ is even, the function $X(N, l, S', L)$ is not vanish, viz. we get "Even Rule".

C. Derivation of a new rule for three equivalent electrons

Based on our theory [equations (1)-(5)], we derived a new rule for three equivalent electrons, which can be stated as a formula below

$$X(3, l, S', L) = \begin{cases} L - \lfloor \frac{L}{3} \rfloor & \text{when } S' = 1, \, 0 \leq L < l \\ l - \lfloor \frac{L}{3} \rfloor & \text{when } S' = 1, \, l \leq L \leq 3l - 1 \\ \lfloor \frac{L}{3} \rfloor - \lfloor \frac{L-l}{2} \rfloor + \lfloor \frac{L-l+1}{2} \rfloor & \text{when } S' = 3, \, 0 \leq L < l \\ \lfloor \frac{L}{3} \rfloor - \lfloor \frac{L-l}{2} \rfloor & \text{when } S' = 3, \, l \leq L \leq 3l - 3 \\ 0 & \text{other cases} \end{cases} \tag{10}$$

This rule can be derived respectively according to the two possible values of S' ($S' = 1$ or 3).

1. *When $S' = 1$*

To $S' = 1$, we will derive the formula below

$$X(3, l, S', L) = \begin{cases} L - \lfloor \frac{L}{3} \rfloor & when \ S' = 1, \ 0 \leq L < l \\ l - \lfloor \frac{L}{3} \rfloor & when \ S' = 1, \ l \leq L \leq 3l - 1 \\ 0 & other \ cases \end{cases} \tag{11}$$

Based on equations (2), (3), and (7), when

$$M'_S = 1, |M_L| \leq f(\frac{3-1}{2} - 1) + f(\frac{3+1}{2} - 1) = 3l - 1,$$

we have

$$A(3, l, l, 1, M_L) = \sum_{M_{L_-}=\{-f(0), \, M_L-f(1)\}_{\max}}^{\{f(0), \, M_L+f(1)\}_{\min}} \{A(1, l, l, 1, M_{L_-})A(2, l, l, 2, M_L - M_{L_-})\}$$

$$= \sum_{M_{L_-}=\{-l, \, M_L-2l+1\}_{\max}}^{\{l, \, M_L+2l-1\}_{\min}} \{(l, M_L - M_{L_-} + l)_{\min} - \lfloor \frac{M_L - M_{L_-}}{2} \rfloor\}$$

$$= \begin{cases} \sum_{M_{L_-}=-l}^{l} \{(l, M_L - M_{L_-} + l)_{\min} - \lfloor \frac{M_L - M_{L_-}}{2} \rfloor\} & \boxed{:A} \\ \sum_{M_{L_-}=M_L-2l+1}^{l} \{l - \lfloor \frac{M_L - M_{L_-}}{2} \rfloor\} & \boxed{:B} \end{cases} \tag{12}$$

where $\boxed{:A}$ here means the case when $0 \leq M_L \leq l - 1$, and $\boxed{:B}$ means the case when $l - 1 \leq M_L \leq 3l - 1$.

Then based on equations (2), (4), and (7), when

$$M'_S = 3, \qquad |M_L| \leq f(2) = 3l - 3,$$

we have

$$A(3, l, l_b, 3, M_L) = \sum_{M_{L_I}=\lfloor \frac{M_L-1}{3} + \frac{3+1}{2} \rfloor}^{\{l_b, \, M_L+f(1)\}_{\min}} A(2, l, M_{L_I} - 1, 2, M_L - M_{L_I})$$

$$= \sum_{M_{L_I}=\lfloor \frac{M_L-1}{3}+2 \rfloor}^{l_b} \left\{ (M_{L_I} - 1, M_L - M_{L_I} + l)_{\min} - \left\lfloor \frac{M_L - M_{L_I}}{2} \right\rfloor \right\} \tag{13}$$

Hence, when $S = 1/2$ $(S' = 1)$, $0 \leq L \leq l - 2$, we have

8

$$\Delta_1 = A(3, l, l, 1, L) - A(3, l, l, 1, L+1)$$

$$= \sum_{M_{L_-}=-l}^{l} \left\{ (l, L - M_{L_-} + l)_{\min} - \lfloor \tfrac{L-M_{L_-}}{2} \rfloor \right\}$$

$$\qquad - \sum_{M_{L_-}=-l}^{l} \left\{ (l, L+1 - M_{L_-} + l)_{\min} - \lfloor \tfrac{L+1-M_{L_-}}{2} \rfloor \right\}$$

$$= \sum_{M_{L_-}=-l}^{l} \left\{ \lfloor \tfrac{L+1-M_{L_-}}{2} \rfloor - \lfloor \tfrac{L-M_{L_-}}{2} \rfloor \right\}$$

$$\qquad + \left(\sum_{M_{L_-}=-l}^{L} + \sum_{M_{L_-}=L+1}^{l} \right) \left\{ (l, L - M_{L_-} + l)_{\min} - (l, L+1 - M_{L_-} + l)_{\min} \right\}$$

$$= \lfloor \tfrac{L+l+1}{2} \rfloor - \lfloor \tfrac{L-l}{2} \rfloor \,^3 + 0 + \sum_{M_{L_-}=L+1}^{l} (-1)$$

$$= \lfloor \tfrac{L+l+1}{2} \rfloor - \lfloor \tfrac{L-l}{2} \rfloor + (L - l) \tag{14}$$

and

$$\Delta_2 = A(3, l, l, 3, L) - A(3, l, l, 3, L+1)$$

$$= \sum_{M_{L_I}=\lfloor \frac{L-1}{3} \rfloor + 2}^{l} \left\{ (M_{L_I} - 1, L - M_{L_I} + l)_{\min} - \lfloor \tfrac{L-M_{L_I}}{2} \rfloor \right\}$$

$$\qquad - \sum_{M_{L_I}=\lfloor \frac{L}{3} \rfloor + 2}^{l} \left\{ (M_{L_I} - 1, L+1 - M_{L_I} + l)_{\min} - \lfloor \tfrac{L+1-M_{L_I}}{2} \rfloor \right\}$$

$$= \left(\sum_{M_{L_I} \le \lfloor \frac{L+l+1}{2} \rfloor} + \sum_{M_{L_I}=\lfloor \frac{L+l+1}{2} \rfloor + 1}^{l} \right) \left\{ (M_{L_I} - 1, L - M_{L_I} + l)_{\min} \right.$$

$$\qquad \left. - (M_{L_I} - 1, L+1 - M_{L_I} + l)_{\min} \right\}$$

$$+ \begin{cases} \displaystyle\sum_{M_{L_I}=\lfloor \frac{L}{3} \rfloor + 2}^{l} \left\{ \lfloor \tfrac{L+1-M_{L_I}}{2} \rfloor - \lfloor \tfrac{L-M_{L_I}}{2} \rfloor \right\} & \boxed{:A} \\[2ex] \displaystyle\sum_{M_{L_I}=\lfloor \frac{L}{3} \rfloor + 2}^{l} \left\{ \lfloor \tfrac{L+1-M_{L_I}}{2} \rfloor - \lfloor \tfrac{L-M_{L_I}}{2} \rfloor \right\} + (\lfloor \tfrac{L-1}{3} \rfloor + 2) - 1 - \lfloor \tfrac{L-(\lfloor \frac{L-1}{3} \rfloor + 2)}{2} \rfloor & \boxed{:B} \end{cases}$$

$$= 0 - \sum_{M_{L_I}=\lfloor \frac{L+l+1}{2} \rfloor + 1}^{l} 1 + \begin{cases} \lfloor \tfrac{L-(\lfloor \frac{L}{3} \rfloor + 2) + 1}{2} \rfloor - \lfloor \tfrac{L-l}{2} \rfloor \,^3 & \boxed{:A} \\[2ex] \lfloor \tfrac{L-(\lfloor \frac{L}{3} \rfloor + 2) + 1}{2} \rfloor - \lfloor \tfrac{L-l}{2} \rfloor \,^3 - \left(\lfloor \tfrac{L}{3} \rfloor - \lfloor \tfrac{L-(\lfloor \frac{L}{3} \rfloor + 1)}{2} \rfloor \right) & \boxed{:B} \end{cases}$$

$$= \lfloor \tfrac{L+l+1}{2} \rfloor - l + \lfloor \tfrac{L}{3} \rfloor - \lfloor \tfrac{L-l}{2} \rfloor \tag{15}$$

Use the formula below (a and b are integers)

[3] $\quad \sum_{i=a}^{b} \left\{ \lfloor \tfrac{i+1}{2} \rfloor - \lfloor \tfrac{i}{2} \rfloor \right\} = \lfloor \tfrac{b+1}{2} \rfloor - \lfloor \tfrac{a}{2} \rfloor$

where $\boxed{:A}$ here means the case when $\frac{L}{3}$ is not an integer, and $\boxed{:B}$ means the case when $\frac{L}{3}$ is an integer. Thus we have

$$
\begin{aligned}
X(3, l, 1, L) = & \ A(3, l, l, 1, L) - A(3, l, l, 1, L+1) \\
& + A(3, l, l, 3, L+1) - A(3, l, l, 3, L) \\
= & \ \Delta_1 - \Delta_2 \\
= & \ L - \left\lfloor \frac{L}{3} \right\rfloor .
\end{aligned} \tag{16}
$$

When $L = l - 1$, according to equation (12), $A(3, l, l, 1, L+1)$ in equation (16) equals

$$
\begin{aligned}
A(3, l, l, 1, l) &= \sum_{M_{L_-}=-l+1}^{l} \{l - \lfloor \frac{l - M_{L_-}}{2} \rfloor\} \\
&= \sum_{M_{L_-}=-l}^{l} \{l - \lfloor \frac{l - M_{L_-}}{2} \rfloor\} - \{l - \lfloor \frac{l - M_{L_-}}{2} \rfloor\} \Big|_{M_{L_-}=-l} \\
&= \sum_{M_{L_-}=-l}^{l} \{l - \lfloor \frac{l - M_{L_-}}{2} \rfloor\},
\end{aligned} \tag{17}
$$

which has the same value as in equation (16). Thus we can get the same expression of function $\mathbf{X}$ also in this case.

When $S = 1/2$ ($S' = 1$), $l \le L \le 3l - 4$, we have

$$
\begin{aligned}
\Delta_1 &= A(3, l, l, 1, L) - A(3, l, l, 1, L+1) \\
&= \sum_{M_{L_-}=L-2l+1}^{l} \left(l - \left\lfloor \frac{L-M_{L_-}}{2} \right\rfloor \right) - \sum_{M_{L_-}=L-2l+2}^{l} \left(l - \left\lfloor \frac{L+1-M_{L_-}}{2} \right\rfloor \right) \\
&= \sum_{M_{L_-}=L-2l+2}^{l} \left\{ \left\lfloor \frac{L+1-M_{L_-}}{2} \right\rfloor - \left\lfloor \frac{L-M_{L_-}}{2} \right\rfloor \right\} + \left(l - \left\lfloor \frac{L-(L-2l+1)}{2} \right\rfloor \right) \\
&= \left(\left\lfloor \frac{L-(L-2l+2)+1}{2} \right\rfloor - \left\lfloor \frac{L-l}{2} \right\rfloor \right) + 1 \\
&= l - \left\lfloor \frac{L-l}{2} \right\rfloor
\end{aligned} \tag{18}
$$

and

$$\Delta_2 = A(3,l,l,3,L) - A(3,l,l,3,L+1)$$

$$= \sum_{M_{L_I}=\lfloor\frac{L-1}{3}\rfloor+2}^{l}\left\{(M_{L_I}-1)-\left\lfloor\frac{L-M_{L_I}}{2}\right\rfloor\right\} - \sum_{M_{L_I}=\lfloor\frac{L}{3}\rfloor+2}^{l}\left\{(M_{L_I}-1)-\left\lfloor\frac{L+1-M_{L_I}}{2}\right\rfloor\right\}$$

$$= \begin{cases} \displaystyle\sum_{M_{L_I}=\lfloor\frac{L}{3}\rfloor+2}^{l}\left\{\left\lfloor\frac{L+1-M_{L_I}}{2}\right\rfloor-\left\lfloor\frac{L-M_{L_I}}{2}\right\rfloor\right\} & \boxed{:A} \\[3mm] \displaystyle\sum_{M_{L_I}=\lfloor\frac{L}{3}\rfloor+2}^{l}\left\{\left\lfloor\frac{L+1-M_{L_I}}{2}\right\rfloor-\left\lfloor\frac{L-M_{L_I}}{2}\right\rfloor\right\}+(\lfloor\frac{L-1}{3}\rfloor+2)-1-\lfloor\frac{L-(\lfloor\frac{L-1}{3}\rfloor+2)}{2}\rfloor & \boxed{:B} \end{cases}$$

$$= \begin{cases} \lfloor\frac{L-(\lfloor\frac{L}{3}\rfloor+2)+1}{2}\rfloor-\lfloor\frac{L-l}{2}\rfloor & \boxed{:A} \\[3mm] \lfloor\frac{L-(\lfloor\frac{L}{3}\rfloor+2)+1}{2}\rfloor-\lfloor\frac{L-l}{2}\rfloor-\left(\lfloor\frac{L}{3}\rfloor-\lfloor\frac{L-(\lfloor\frac{L}{3}\rfloor+1)}{2}\rfloor\right) & \boxed{:B} \end{cases}$$

$$= \lfloor\tfrac{L}{3}\rfloor - \lfloor\tfrac{L-l}{2}\rfloor \tag{19}$$

where $\boxed{:A}$ here means the case when $\frac{L}{3}$ is not an integer, and $\boxed{:B}$ means the case when $\frac{L}{3}$ is an integer. Thus we have

$$\begin{aligned} X(3,l,1,L) =\ & A(3,l,l,1,L) - A(3,l,l,1,L+1) \\ & + A(3,l,l,3,L+1) - A(3,l,l,3,L) \\ =\ & \Delta_1 - \Delta_2 \\ =\ & l - \lfloor\tfrac{L}{3}\rfloor. \end{aligned} \tag{20}$$

When $L = 3l-3$, $A(3,l,l,3,L+1)$ vanishes; when $L = 3l-2$, $A(3,l,l,3,L)$ also vanishes; when $L = 3l-1$, $A(3,l,l,1,L+1)$ also vanishes; and we can get the function $\mathbf{X}$ which equals 1, coinciding with equation (20).

Combining equations (16) and (20), we get the equation (11).

2. When $S' = 3$

To $S' = 3$, we will derive the formula below

$$X(3,l,S',L) = \begin{cases} \lfloor\frac{L}{3}\rfloor - \lfloor\frac{L-l}{2}\rfloor + \lfloor\frac{L-l+1}{2}\rfloor & when\ S'=3,\ 0\le L<l-1 \\[2mm] \lfloor\frac{L}{3}\rfloor - \lfloor\frac{L-l}{2}\rfloor & when\ S'=3,\ l-1\le L\le 3l-3 \\[2mm] 0 & other\ cases \end{cases} \tag{21}$$

11

Based on equations (15), when

$$S = 3/2 \ (S' = 3), \ 0 \le L \le l - 1,$$

we have

$$
\begin{aligned}
\Delta_1 &= A(3, l, l, 3, L) - A(3, l, l, 3, L+1) \\
&= \left\lfloor \frac{L - l + 1}{2} \right\rfloor + \lfloor \frac{L}{3} \rfloor - \left\lfloor \frac{L - l}{2} \right\rfloor
\end{aligned}
\tag{22}
$$

Δ_2 just vanishes, thus we have

$$
\begin{aligned}
X(3, l, 3, L) &= A(3, l, l, 3, L) - A(3, l, l, 3, L+1) \\
&\quad + A(3, l, l, 5, L+1) - A(3, l, l, 5, L) \\
&= \Delta_1 - \Delta_2 \\
&= \lfloor \frac{L}{3} \rfloor - \lfloor \frac{L-l}{2} \rfloor + \lfloor \frac{L-l+1}{2} \rfloor
\end{aligned}
\tag{23}
$$

Based on equations (19), when

$$S = 3/2 \ (S' = 3), \ l \le L \le 3l - 4,$$

we have

$$
\Delta_1 = A(3, l, l, 3, L) - A(3, l, l, 3, L+1) = \left\lfloor \frac{L}{3} \right\rfloor - \left\lfloor \frac{L - l}{2} \right\rfloor
\tag{24}
$$

When $L = 3l - 3$, $A(3, l, l, 3, L+1)$ vanishes, and we can get the function Δ_1 equaling 1, which also can be expressed by equation (24). Δ_2 also vanishes, thus we have

$$
\begin{aligned}
X(3, l, 3, L) &= A(3, l, l, 3, L) - A(3, l, l, 3, L+1) \\
&\quad + A(3, l, l, 5, L+1) - A(3, l, l, 5, L) \\
&= \Delta_1 - \Delta_2 \\
&= \lfloor \frac{L}{3} \rfloor - \lfloor \frac{L-l}{2} \rfloor
\end{aligned}
\tag{25}
$$

Combining equations (23) and (25), we get the equation (21). Banding together both of equations (11) and (21), we naturally get the rule for three equivalent electrons [equation (10)].

V. CONCLUSION

Mainly based on a digital counting procedure, the alternative mathematical technique to determine the LS spectral terms arising from l^N configurations, is immediately applicable for studies involving one orbital shell model. It makes the calculation of coupled states of excited high energy electrons possible, and offered a basis for the further calculations of energy levels for laser and soft X-ray. Though the derivation of our theory is a little complicated and thus is presented in Appendix below. Compared to other theoretical methods reported earlier in literature, this method is much more compact, and especially offered a direct way in calculation.

In addition, based on this alternative mathematical basis, we may also try to calculate the statistical distribution of J-values for l^N configurations [20], and try to deduce some more powerful rules or formulas probably could be deduced for determining the LS terms, such as equations (9) and (10). Indeed, it may also be applicable to other coupling schemes.

APPENDIX A: DERIVATION OF THE MAIN FORMULA EQUATION (1)

Now we'll determine the number of spectral terms having total orbital angular quantum number L and total spin quantum number $S'/2$ arising from l^N electronic configurations, which is denoted by $X(N, l, S', L)$.

The number of spectral terms having allowed orbital magnetic quantum number L_0 and spin magnetic quantum number $S'_0/2$ in l^N electronic configurations equals $A(N, l, l, S'_0, L_0)$, namely the number of spectral terms with $L \geq L_0$, $S \geq S'_0/2$. And these spectral terms can also be subdivided according to their quantum numbers of L and S into four types as follows:

①. $L = L_0, S = S'_0/2$: the number of this type is $X(N, l, S'_0, L_0)$.

②. $L = L_0, S \geq \frac{S'_0}{2} + 1$: the number of this type equals

$$A(N, l, l, S'_0 + 2, L_0) - A(N, l, l, S'_0 + 2, L_0 + 1).$$

③. $L \geq L_0 + 1, S = S'_0/2$: the number of this type equals

$$A(N, l, l, S'_0, L_0 + 1) - A(N, l, l, S'_0 + 2, L_0 + 1).$$

④. $L \geq L_0 + 1, S \geq \frac{S'_0}{2} + 1$: the number of this type is $A(N, l, l, S'_0 + 2, L_0 + 1)$.

Hence, we have

$$A(N, l, l, S'_0, L_0) = X(N, l, S'_0, L_0) + A(N, l, l, S'_0 + 2, L_0 + 1)$$
$$+ \{A(N, l, l, S'_0 + 2, L_0) - A(N, l, l, S'_0 + 2, L_0 + 1)\}$$
$$+ \{A(N, l, l, S'_0, L_0 + 1) - A(N, l, l, S'_0 + 2, L_0 + 1)\}. \tag{A1}$$

Therefore

$$X(N, l, S', L) = A(N, l, l, S', L) + A(N, l, l, S' + 2, L + 1) - A(N, l, l, S' + 2, L)$$
$$- A(N, l, l, S', L + 1). \tag{A2}$$

APPENDIX B: DERIVATION OF EQUATION (2)

For one-particle configurations $(N = 1)$, there is only one spectral term. Thus toward any allowable value of M_L, we have

$$A(1, l, l_b, 1, M_L) = 1 \qquad (-l \leq M_L \leq l). \tag{B1}$$

APPENDIX C: DERIVATION OF EQUATION (3)

In this case $(N \geq 2)$, there are some electrons spin-up and others spin-down. Taking account of the Pauli principle, we sort the N electrons into two classes: (1) Spin-down electrons class $\ominus$ consists of k_- (≥ 1) electrons with $m_{s_i} = -1/2$ ($i = 1, 2, \ldots, k_-$); (2) Spin-up electrons class $\oplus$ consists of k_+ (≥ 1) electrons with $m_{s_j} = 1/2$ ($j = 1, 2, \ldots, k_+$). In each class, the orbital magnetic quantum number of each electron is different from each other. The total spin and orbital magnetic quantum number for class $\ominus$ are

$$M_{s_-} = \sum_{i=1}^{k_-} m_{s_i} = -\frac{k_-}{2} \qquad M_{L_-} = \sum_{i=1}^{k_-} m_{l_i}. \tag{C1}$$

For class $\oplus$,

$$M'_{s_+} = 2M_{s_+} = 2\sum_{j=1}^{k_+} m_{s_j} = k_+ \qquad M_{L_+} = \sum_{j=1}^{k_+} m_{l_j}. \tag{C2}$$

1. The number of permitted states to each M_{L_-} value

When M_L is fixed, for each allowable value of M_{L_-}, there is a unique corresponding value of $M_{L_+} = M_L - M_{L_-}$. We can denote by $A(k_-, l, l, M'_{s_-}, M_{L_-})$ the number of permitted states of the k_- electrons in class $\ominus$ according to the notations defined in Section II. Based on any LS term having a spin magnetic quantum number M_S must also have a spin magnetic quantum number $-M_S$, we have

$$
\begin{aligned}
A(k_-, l, l, M'_{s_-}, M_{l_-}) &= A(k_-, l, l, -M'_{s_-}, M_{l_-}) \\
&= A(k_-, l, l, k_-, M_{l_-}).
\end{aligned}
\tag{C3}
$$

Correspondingly we denote by $A(k_+, l, l, M'_{s_+}, M_{L_+}) = A(k_+, l, l, k_+, M_L - M_{L_-})$ for class $\oplus$. Hence, to any value of M_{L_-}, the total number of permitted states of l^N is $A(k_-, l, l, k_-, M_{L_-})\, A(k_+, l, l, k_+, M_L - M_{L_-})$.

2. Determination of the range of M_{L_-}

Firstly, the value of $\sum_{i=1}^{k_-} m_{l_i}$ is minimum, when the orbital magnetic quantum numbers of the k_- electrons in class $\ominus$ respectively are $-l, -(l-1), \ldots, -(l-k_-+1)$. Thus we have

$$
(M_{L_-})_{\min} \geq \left(\sum_{i=1}^{k_-} m_{l_i}\right)_{\min} = -\sum_{m=0}^{k_--1}(l-m).
\tag{C4}
$$

Similarly, the value of $\sum_{j=1}^{k_+} m_{l_j}$ is maximum, when the orbital magnetic quantum numbers of the k_+ electrons in class $\oplus$ respectively are $l, (l-1), \ldots, (l-k_++1)$. Thus we have

$$
(M_{L_-})_{\min} \geq M_L - (M_{L_+})_{\max} = M_L - \sum_{m=0}^{k_+-1}(l-m).
\tag{C5}
$$

Comparing the equation (C4) with equation (C5), we have

$$
(M_{L_-})_{\min} = \left\{ -\sum_{m=0}^{k_--1}(l-m), \ M_L - \sum_{m=0}^{k_+-1}(l-m) \right\}_{\max}
\tag{C6}
$$

Similarly, due to

$$
(M_{L_-})_{\max} \leq \left(\sum_{i=1}^{k_-} m_{l_i}\right)_{\max} = \sum_{m=0}^{k_--1}(l-m),
\tag{C7}
$$

$$
(M_{L_-})_{\max} \leq M_L - (M_{L_+})_{\min} = M_L + \sum_{m=0}^{k_+-1}(l-m),
\tag{C8}
$$

we have

$$(M_{L_-})_{\max} = \left\{ \sum_{m=0}^{k_- -1} (l-m), \ M_L + \sum_{m=0}^{k_+ -1} (l-m) \right\}_{\min} \tag{C9}$$

3. The total number of permitted states

Recalling the relationship among k_+, k_- and M_S', N,

$$\begin{cases} N = k_+ + k_-, & \text{(C10)} \\[2mm] M_S' = 2M_S = 2M_{s_-} + 2M_{s_+} = k_+ - k_-, & \text{(C11)} \end{cases}$$

we have

$$k_- = (N - M_S')/2 \qquad k_+ = (N + M_S')/2. \tag{C12}$$

Consequently, we get

$$A(N,l,l,M_S',M_L) = \sum_{M_{L_-}=(M_{L_-})_{\min}}^{(M_{L_-})_{\max}} \left\{ A(k_-,l,l,k_-,M_{L_-}) \ A(k_+,l,l,k_+,M_L - M_{L_-}) \right\}$$

$$= \sum_{M_{L_-}=\{-f(\frac{N-M_S'}{2}-1), \ M_L-f(\frac{N+M_S'}{2}-1)\}_{\max}}^{\{f(\frac{N-M_S'}{2}-1), \ M_L+f(\frac{N+M_S'}{2}-1)\}_{\min}} \left\{ A(\tfrac{N-M_S'}{2},l,l,\tfrac{N-M_S'}{2},M_{L_-}) \right.$$

$$\left. \times A(\tfrac{N+M_S'}{2},l,l,\tfrac{N+M_S'}{2},M_L - M_{L_-}) \right\}. \tag{C13}$$

4. The domain of definition

a. The range of M_L and L

Based on

$$(M_{L_-})_{\min} + (M_{L_+})_{\min} \leqslant M_L \leqslant (M_{L_-})_{\max} + (M_{L_+})_{\max}, \tag{C14}$$

and

$$(M_{L_\pm^+})_{\min} = -\sum_{m=0}^{k_-^+ -1} (l-m), \ (M_{L_\pm^+})_{\max} = \sum_{m=0}^{k_-^+ -1} (l-m), \tag{C15}$$

we have

$$|M_L| \leqslant f\left(\frac{N - M_S'}{2} - 1\right) + f\left(\frac{N + M_S'}{2} - 1\right). \tag{C16}$$

Therefore, the total orbital angular quantum number L must fulfil the inequality

$$0 \leqslant L \leqslant f\left(\frac{N - M_S'}{2} - 1\right) + f\left(\frac{N + M_S'}{2} - 1\right). \tag{C17}$$

16

b. The range of M_S' and S'

Concerning

$$M_S' = k_+ - k_- = k_+ - (N - k_+) = 2k_+ - N, \tag{C18}$$

$$(k_+)_{\min} = 1 \qquad (k_+)_{\max} = N - 1, \tag{C19}$$

we have

$$\{M_S'\} = \{2 - N, 4 - N, \ldots, N - 4, N - 2\}. \tag{C20}$$

and

$$\{S'\} = \begin{cases} \{0, 2, \ldots, N - 2\} & (\text{N even}) \\ \{1, 3, \ldots, N - 2\} & (\text{N odd}) \end{cases} \tag{C21}$$

Now we reduce the two expressions into one expression

$$\{S'\} = \{N - 2\lfloor N/2 \rfloor, N + 2 - 2\lfloor N/2 \rfloor, \ldots, N - 2\}. \tag{C22}$$

Therefore, the equation (3) has been proved completely.

APPENDIX D: DERIVATION OF EQUATION (4)

Now we discuss the case that all of the N electrons are spin-up, namely

$$M_S' = N \quad and \quad M_S = N/2. \tag{D1}$$

Based on the Pauli exclusion principle, we can prescribe

$$m_{l_1} > m_{l_2} > \ldots > m_{l_i} > \ldots > m_{l_N}. \tag{D2}$$

Now we also treat these electrons as two classes: (1) Class ① consists of the electron whose orbital magnetic quantum number is largest; (2) Class ⑪ consists of the other electrons. Thus the total orbital magnetic quantum number of the two classes are

$$M_{L_I} = m_{l_1} \qquad M_{L_{II}} = \sum_{i=2}^{N} m_{l_i} \tag{D3}$$

1. The number of permitted states to each M_{L_I} value

In view of inequality (D2), we have

$$(m_{l_{i+1}})_{\max} = m_{l_i} - 1 \qquad (i = 1, 2, \ldots, N - 1). \tag{D4}$$

Thus we can denote by $A(N - 1, l, l_b, N - 1, M_{L_{II}})$ which equals $A(N - 1, l, M_{L_I} - 1, N - 1, M_L - M_{L_I})$, the permitted states of class ⑪ consisting of the latter $(N - 1)$ electrons, according to the notations prescribed in Section II. For any allowed value of M_{L_I}, there is only one state for class ①. Therefore, to each value of M_{L_I}, the total number of permitted states of the N electrons is $A(N - 1, l, M_{L_I} - 1, N - 1, M_L - M_{L_I})$.

Then in class ⑪, we can treat m_{l_2} as M_{L_I}, and the latter $(\sum_{i=3}^{N} m_{l_i})$ as $M_{L_{II}}, \ldots$. Just continue our operation in this way, after $(N - 1)$ times of operation, and then based on equation (2), we can get the final value of $A(N, l, l_b, N, M_L)$.

2. The range of M_{L_I}

Based on

$$(M_{L_I})_{\max} \leqslant M_L - (M_{L_{II}})_{\min} = M_L + \sum_{m=0}^{N-2} (l - m), \tag{D5}$$

$$(M_{L_I})_{\max} \leqslant l_b, \tag{D6}$$

we have

$$(M_{L_I})_{\max} = \{l_b, \ M_L + \sum_{m=0}^{N-2} (l - m)\}_{\min}. \tag{D7}$$

In the following, we will prove

$$(M_{L_I})_{\min} = \lfloor \frac{M_L - 1}{N} + \frac{N + 1}{2} \rfloor. \tag{D8}$$

Because of the symmetrical situation between $M_L > 0$ and $M_L < 0$ to a certain LS term, it is necessary only to consider the part of the case which corresponds to $M_L \geq 0$.

In the case of M_{L_I} being minimum, we have

$$(m_{l_2})_{\min} = M_{L_I} - 2, \ (m_{l_{i+1}})_{\min} = m_{l_i} - 1, \tag{D9}$$

where (i=2,...,N-1). Based on equations (D4) and (D9), we get the maximum value of M_L

$$
\begin{aligned}
(M_L)_{\max} &= (M_{L_I})_{\min} + (M_{L_{II}})_{\max} \\
&= (M_{L_I})_{\min} + \sum_{i=2}^{N}\{(M_{L_I})_{\min} - (i-1)\} \\
&= N(M_{L_I})_{\min} - \frac{N(N-1)}{2};
\end{aligned}
\tag{D10}
$$

and the minimum value of M_L

$$
\begin{aligned}
(M_L)_{\min} &= (M_{L_I})_{\min} + (M_{L_{II}})_{\min} \\
&= (M_{L_I})_{\min} + \sum_{i=2}^{N}\{(M_{L_I})_{\min} - i\} \\
&= N(M_{L_I})_{\min} - \frac{N(N-1)}{2} - (N-1).
\end{aligned}
\tag{D11}
$$

Therefore

$$
M_L = N(M_{L_I})_{\min} - \frac{N(N-1)}{2} - j,
\tag{D12}
$$

$$
(M_{L_I})_{\min} = \frac{M_L + j}{N} + \frac{N-1}{2},
\tag{D13}
$$

where j could be $0, 1, \ldots,$ and $N-1$, which just to make sure that $(M_{L_I})_{\min}$ is an integer. Thus

$$
(M_{L_I})_{\min} = \lfloor \frac{M_L + N - 1}{N} + \frac{N-1}{2} \rfloor = \lfloor \frac{M_L - 1}{N} + \frac{N+1}{2} \rfloor.
\tag{D14}
$$

Consequently, we get

$$
\begin{aligned}
A(N, l, l_b, N, M_L) &= \sum_{M_{L_I}=(M_{L_I})_{\min}}^{(M_{L_I})_{\max}} A(N-1, l, M_{L_I} - 1, N-1, M_L - M_{L_I}) \\
&= \sum_{M_{L_I}=\lfloor \frac{M_L-1}{N}+\frac{N+1}{2} \rfloor}^{\{l_b,\, M_L+\sum_{m=0}^{N-2}(l-m)\}_{\min}} A(N-1, l, M_{L_I} - 1, N-1, M_L - M_{L_I})
\end{aligned}
\tag{D15}
$$

3.   The range of M_L and L

Based on

$$
(M_L)_{\min} = -\sum_{m=0}^{N-1}(l - m) \qquad (M_L)_{\max} = \sum_{m=0}^{N-1}(l - m),
\tag{D16}
$$

19

we have

$$|M_L| \leqslant f(N-1). \tag{D17}$$

Hence the total orbital angular quantum number L must fulfil

$$0 \leqslant L \leqslant f(N-1). \tag{D18}$$

So, the equation (4) has been proved completely.

Now we have completely proved the five formulas represented in Section II.

ACKNOWLEDGMENTS

[1] I. M. Gelfand and M. I. Graev, Izv. Akad. Nauk SSSR Ser. Mat. **29**, 1329 (1965) (in Russian); English translation: I. M. Gelfand and M. I. Graev, Amer. Math. Soc. Transl. Ser. II **64**, 116 (1965).

[2] M. Moshinsky, *Rev. Mod. Phys.* **34**, 813 (1962); M. Moshinsky, *J. Math. Phys.* **4**, 1128 (1963); M. Moshinsky, *Group Theory and the Many-Body Problems* (Gordon and Breach, New York, 1968); J. G. Nagel and M. Moshinsky, *J. Math. Phys.* **6**, 682 (1965).

[3] L. C. Biedenharn, *J. Math. Phys.* **4**, 436 (1963a); G. E. Braid and L. C. Biedenharn, *J. Math. Phys.* **4**, 1449 (1963b); G. E. Braid and L. C. Biedenharn, *J. Math. Phys.* **5**, 1723 (1964a); G. E. Braid and L. C. Biedenharn, *J. Math. Phys.* **5**, 1730 (1964b); G. E. Braid and L. C. Biedenharn, *J. Math. Phys.* **6**, 1847 (1965); L. C. Biedenharn, A. Giovanini and J. D. Louck, *J. Math. Phys.* **8**, 691 (1967).

[4] B. R. Judd, *Phys. Rev.* **162**, 28 (1967).

[5] J. D. Louck, *J. Math. Phys.* **6**, 1786 (1965); J. D. Louck, *Am. J. Phys.* **38**, 3 (1970a); J. D. Louck and L. C. Biedenharn, *J. Math. Phys.* **11**, 2386 (1970b); J. D. Louck and L. C. Biedenharn, *J. Math. Phys.* **14**, 1336 (1973).

[6] J. Drake, G. W. F. Drake and M. Schlesinger, *J. Phys. B* **8**, 1009 (1975); G. W. F. Drake and M. Schlesinger, *Phys. Rev. A* **15**, 1990 (1977).

[7] W. G. Harter, *Phys. Rev. A* **8**, 2819 (1973); W. G. Harter and C. W. Patterson, *Phys. Rev. A* **13**, 1067 (1976); C. W. Patterson and W. G. Harter, *Phys. Rev. A* **15**, 2372 (1977).

[8] J. Paldus, *Phys. Rev. A* **14**, 1620 (1976).

[9] J. Paldus, *J. Chem. Phys. A* **61**, 5321 (1974).

[10] D. Braunschweig and K.T. Hecht, *J. Math. Phys.* **19**, 720 (1978).

[11] R. D. Kent and M. Schlesinger, *Phys. Rev. A* **23**, 979 (1981).

[12] H. Weyl, *The Classical Groups, Their Invariants and Representations* (Princeton Univ. Press, Princeton, 1939); H. Weyl, *The Theory of Groups and Quantum Mechanics* (Dover, New York, 1931).

[13] G. Racah, *Phys. Rev.* **61**, 186 (1942a); G. Racah, *Phys. Rev.* **62**, 438 (1942b); G. Racah, *Phys. Rev.* **63**, 367 (1943); G. Racah, *Phys. Rev.* **76**, 1352 (1949).

[14] S. Meshkov, *Phys. Rev.* **91**, 871 (1953).

[15] R. D. Cowan, *The Theory of Atomic Structure and Spectra* (Univ. California Press, Berkeley, CA, 1981).

[16] H. N. Russell, *Phys. Rev.* **29**, 782 (1927).

[17] H. N. Russell, and F.A. Saunders, *Astrophys. J.* **61**, 40 (1925).

[18] R. C. Gibbs, D.T. Willber and H.E. White, *Phys. Rev.* **29**, 790 (1927).

[19] E. U. Condon and G.H. Shortley, *The Theory of Atomic Spectra* (Cambridge Univ. Press, Cambridge, 1979).

[20] J. Bauche and P. Cossé, *J. Phys. B: At. Mol. Opt. Phys.* **30**, 1411 (1997).