

RESEARCH ARTICLE | AUGUST 01 1965

Atomic Terms for Equivalent Electrons

N. Karayianis



J. Math. Phys. 6, 1204–1209 (1965)

<https://doi.org/10.1063/1.1704761>



Articles You May Be Interested In

Lie transformations, similarity reduction, and solutions for the nonlinear Madelung fluid equations with external potential

J. Math. Phys. (June 1987)

Application of double Gel'fand polynomials to the symmetric group and spin–isospin wave functions of cluster systems

J. Math. Phys. (October 1984)



AIP Advances

Why Publish With Us?

**21DAYS**
average time
to 1st decision

**OVER 4 MILLION**
views in the last year

**INCLUSIVE**
scope

[Learn More](#)

 AIP
Publishing

Atomic Terms for Equivalent Electrons

N. KARAYIANIS

Harry Diamond Laboratories, Washington, D. C.

(Received 18 August 1964; final manuscript received 1 October 1964)

The problem of determining the number of times, $b(l N L S)$, a given term occurs in an atomic configuration of the form $(nl)^N$ is considered by the methods of group theory. The b are shown to be related to the classical problem of partitioning numbers. Several expressions relating b to other, simpler partitions are obtained, which result in a recursion relationship for the b . A table for $b(4 N L S)$ is included to complement existing tables for the range $1 \leq l \leq 3$, which are found in several places in the literature.

I. INTRODUCTION

THE restriction of atomic wavefunctions to those that are antisymmetric on the interchange of any two electrons limits the possible Russell-Saunders (LS) states for a given atomic configuration. The limitation is especially pronounced for configurations of the form $(nl)^N$, i.e., for equivalent electrons, because the full burden of antisymmetrization must be absorbed by the angular momentum variables—the only way in which the single-electron states may differ in these configurations. For two equivalent electrons, the allowed terms are those for which $L + S = \text{even}$, and each such term is found to occur just once. For an arbitrary number of equivalent electrons, the manner in which antisymmetrization manifests itself cannot, however, be so simply expressed. One finds that the number of times, $b(l N L S)$ [hereafter written $b(l N L S)$ for conciseness], a given LS term appears increases rapidly as l (the orbital angular momentum of each electron) and N (the number of electrons) increase, and moreover, for fixed l , N , and S , the number of terms as L varies, fluctuates irregularly. The $b(l N L S)$, on the other hand, are not dependent on the principal quantum number n , provided n is greater than l .

The problem of determining the numbers $b(l N L S)$ dates back to Breit¹ in 1926. The following year, Russell² and Gibbs, Wilber, and White³ simultaneously published results extending Breit's algorithm to obtain the b for all possible configurations involving p , d , and f electrons. The method developed by Breit relies on a manipulation of the angular momentum projections (the so-called "magnetic quantum numbers") of single electron states and is very laborious in spite of the improvements by

the other authors. A good summary of the method is given by White.⁴

Recently, Curl and Kilpatrick⁵ treated the same problem by the more elegant methods of group theory. They obtained a generating function $J_s(x)$ that generates the desired quantities in the form

$$J_s(x) = \sum_L b(l N L S)(x^L - x^{-L-1}). \quad (1)$$

The contribution of Curl and Kilpatrick represents a significant improvement over Breit's method for obtaining the b even though, in practice, the process for finding a given b by expanding $J_s(x)$ in powers of x may still involve much labor.

A consideration of the known methods for determining the b indicates that these quantities are related to the classical problem of partitioning numbers, i.e., the problem of determining the number of unique ways an integer can be expressed as a summation over a set of other integers restricted by certain conditions. The method of Breit, particularly, gives a strong indication of this relationship. One may, therefore, reasonably expect the b to exhibit properties generally shared by the various partitions that have been studied.⁶ Among these properties are (1) each partition is associated with a relatively simple generating function, (2) each satisfies a recursion relationship, and (3) there exist interconnecting formulas relating the various partitions. Only one of these properties, the first, has been found previously in connection with the b 's. Owing to the facility with which tables for a given partition can be obtained using the recursion rela-

¹ G. Breit, *Phys. Rev.* **28**, 334 (1926).

² H. N. Russell, *Phys. Rev.* **29**, 782 (1927).

³ R. C. Gibbs, D. T. Wilber, and H. E. White, *Phys. Rev.* **29**, 790 (1927).

⁴ H. E. White, *Introduction to Atomic Spectra* (McGraw-Hill Book Company, Inc., New York, 1934), 1st ed., pp. 235, 293, and 437.

⁵ R. F. Curl, Jr., and J. E. Kilpatrick, *Am. J. Phys.* **28**, 357 (1960).

⁶ H. Gupta, *Royal Society Mathematical Tables, Partitions* 4 (Cambridge University Press, Cambridge, England, 1958).

TABLE I. Values for $b(4NLS)$ in the range $2 \leq N \leq 5$, $0 \leq L$, and $0 \leq S$. All b for arguments in this range not given in the table are zero.

L	$N = 2$		$N = 3$		$N = 4$			$N = 5$		
	$S = 1$	$S = 0$	$S = \frac{1}{2}$	$S = \frac{1}{2}$	$S = 2$	$S = 1$	$S = 0$	$S = 5/2$	$S = 3/2$	$S = 1/2$
0	0	1	0	0	1	0	3	1	1	3
1	1	0	1	1	0	4	0	0	4	5
2	0	1	0	2	2	3	5	2	6	10
3	1	0	2	2	1	6	2	1	8	11
4	0	1	1	3	2	5	6	2	9	15
5	1	0	1	3	1	7	3	1	9	14
6	0	1	1	2	2	5	6	2	9	15
7	1	0	1	2	1	6	3	1	8	13
8	0	1	0	2	1	4	5	1	7	13
9			1	1	0	4	2	0	6	10
10			0	1	1	2	3	1	4	9
11			0	1	0	2	1	0	3	6
12					0	1	2	0	2	5
13					0	1	0	0	1	3
14					0	0	1	0	1	2
15								0	0	1
16								0	0	1

tionship it satisfies, it is desirable to find such a relationship for b .

This paper reports the results of a successful investigation towards this end. In addition to obtaining a recursion relationship for the b , several new formulas are obtained relating this quantity to other, simpler partitions. Finally, the generating function of Curl and Kilpatrick and a new generating function related to it are derived for completeness.

The recursion relationship for b , given by (22) in Sec. III of this paper, lends itself well to computer calculations. A table for $b(4NLS)$ for all values of N , L , and S , and for l in the range $1 \leq l \leq 6$ was obtained in this manner and is available upon

request.⁷ The values for $l = 4$ are included in this paper in Tables I, II, and III to complement existing tables found in the literature.³⁻⁵

II. A REDUCIBLE REPRESENTATION

Consider the finite-dimensional linear vector space Γ comprising the antisymmetric wavefunctions of N equivalent electrons, each with orbital angular momentum l . This space is invariant with respect to the three-dimensional rotation operators in coordinate space, $R_L = \exp(-in \cdot L\theta)$, and in spin space, $R_S = \exp(-in' \cdot S\phi)$, where $L = \sum_1^N l_i$ and $S = \sum_1^N s_i$. As a result of this invariance, Γ is a carrier of a representation for the product group formed

TABLE II. Values for $b(4NLS)$ in the range $6 \leq N \leq 7$, $0 \leq L$, and $0 \leq S$. All b for arguments in this range not given in the table are zero.

L	$N = 6$				$N = 7$			
	$S = 3$	$S = 2$	$S = 1$	$S = 0$	$S = 7/2$	$S = 5/2$	$S = 3/2$	$S = 1/2$
0	0	2	1	7	0	1	2	5
1	1	3	13	3	1	3	13	15
2	0	8	13	13	0	5	16	24
3	2	7	23	11	1	6	25	31
4	1	10	21	19	0	7	25	37
5	1	9	28	13	1	7	30	39
6	1	10	23	21	0	7	27	40
7	1	8	26	14	1	6	28	39
8	0	8	20	17	0	5	23	36
9	1	5	20	12	0	4	22	32
10	0	5	14	13	0	3	16	27
11	0	3	13	7	0	2	14	22
12	0	2	8	9	0	1	9	17
13	0	1	7	4	0	1	7	13
14	0	1	3	4	0	0	4	9
15	0	0	3	2	0	0	3	6
16	0	0	1	2	0	0	1	4
17	0	0	1	0	0	0	1	2
18	0	0	0	1	0	0	0	1
19					0	0	0	1

⁷ N. Karayianis and Arthur Hausner, HDL Report No. R-RCB-64-1, June 1964.

TABLE III. Values for $b(4NLS)$ in the range $8 \leq N \leq 9$, $0 \leq L$, and $0 \leq S$.
All b for arguments in this range not given in the table are zero.

L	$N=8$ $S=4$	$S=3$	$S=2$	$S=1$	$S=0$	$N=9$ $S=9/2$	$S=7/2$	$S=5/2$	$S=3/2$	$S=1/2$
0	0	0	5	3	10	1	0	3	6	8
1	0	2	7	23	7	0	1	3	16	19
2	0	2	16	27	24	0	1	9	24	35
3	0	4	16	43	20	0	1	8	34	40
4	1	3	22	43	34	0	1	12	38	52
5	0	4	20	53	28	0	1	10	40	54
6	0	3	23	48	37	0	1	12	42	56
7	0	3	19	52	28	0	1	9	39	53
8	0	2	19	43	34	0	1	9	35	53
9	0	2	14	42	24	0	0	6	32	44
10	0	1	13	32	26	0	0	6	26	40
11	0	1	8	29	17	0	0	3	20	32
12	0	0	7	20	18	0	0	3	16	26
13	0	0	4	17	10	0	0	1	11	19
14	0	0	3	10	10	0	0	1	7	15
15	0	0	1	8	5	0	0	0	5	9
16	0	0	1	4	5	0	0	0	3	7
17	0	0	0	3	2	0	0	0	1	4
18	0	0	0	1	2	0	0	0	1	2
19	0	0	0	1	0	0	0	0	0	1
20	0	0	0	0	1	0	0	0	0	1

by the operators $R_L R_S$. The reduction of this representation into its irreducible components provides the number of states, $b(4NLS)$, which belong simultaneously to the $(2L+1)$ -dimensional irreducible representation of the rotation group in coordinate space and the $(2S+1)$ -dimensional irreducible representation of the rotation group in spin space.

Let the matrix representation for $R_L R_S$ in terms of some basis in Γ be given by $D(R_L R_S)$. Further, let U represent the unitary transformation that effects the reduction of D as follows,

$$UD(R_L R_S)U^{-1} = \sum_{L'S'} b(4NL'S') D^{2L'+1}(R_L) \times D^{2S'+1}(R_S), \quad (2)$$

where the D matrices on the right-hand side are irreducible representations of the respective three-dimensional rotation groups. Taking traces of both sides, one has

$$\text{Tr}[D(R_L R_S)] = \sum_{L'S'} b(4NL'S') \chi^{2L'+1}(R_L) \chi^{2S'+1}(R_S), \quad (3)$$

where the χ are characters of the respective rotations in the given irreducible representations.

To evaluate (3), it is sufficient to choose the rotations

$$R_L = e^{-iL_z \theta}, \quad R_S = e^{-iS_z \varphi}, \quad (4)$$

for which the characters are given by the well-known expressions

$$\chi^{2L'+1}(R_L) = \sin(L' + \frac{1}{2})\theta / \sin \frac{1}{2}\theta, \quad (5)$$

$$\chi^{2S'+1}(R_S) = \sin(S' + \frac{1}{2})\varphi / \sin \frac{1}{2}\varphi.$$

The trace of $D(R_L R_S)$ may be evaluated by choosing any convenient orthonormal basis in Γ . We choose the set of determinantal wavefunctions u , that are known to span Γ and to be diagonal in L_z and S_z . The u , are antisymmetrized product wavefunctions of the N single-electron states. A typical matrix element for $R_L R_S$ in this basis is

$$u_{\lambda}^{\dagger} R_L R_S u_{\lambda} = D_{\nu\lambda}(e^{-iL_z \theta} e^{-iS_z \varphi}) = \delta_{\nu\lambda} e^{-iM_L(\nu)\theta} e^{-iM_S(\nu)\varphi}, \quad (6)$$

where $M_L(\nu) = \sum_1^N m_i$ and $M_S(\nu) = \sum_1^N \mu_i$, and the m_i and μ_i are respectively the individual z projections of the orbital angular momentum and spin for the single-electron states. The trace of $D(R_L R_S)$ is then given by

$$\text{Tr}[D(R_L R_S)] = \sum_{M_L M_S} A(M_L M_S) e^{-iM_L \theta} e^{-iM_S \varphi}, \quad (7)$$

where $A(M_L M_S)$ represents the number of determinantal wavefunctions for a given M_L and M_S . Equating (3) and (7), and substituting the character values given by (5), one obtains

$$\sum_{L'S'} b(4NL'S') \sin(L' + \frac{1}{2})\theta \sin(S' + \frac{1}{2})\varphi = \sum_{M_L M_S} A(M_L M_S) \sin \frac{1}{2}\theta \sin \frac{1}{2}\varphi e^{-iM_L \theta} e^{-iM_S \varphi}. \quad (8)$$

The summation on the left is restricted to $L' \geq 0$, $S' \geq 0$, whereas M_L and M_S assume positive and

negative values. Owing to the fact A is even in both M_L and M_S , operating on (8) with

$$(\pi)^{-2} \int_0^{2\pi} d\theta \int_0^{2\pi} d\varphi \sin(L + \frac{1}{2})\theta \sin(S + \frac{1}{2})\varphi \quad (9)$$

gives the result

$$b(lNLS) = \sum_{\lambda\sigma} (-)^{\lambda+\sigma} \binom{1}{\lambda} \binom{1}{\sigma} A(L + \lambda, S + \sigma). \quad (10)$$

Considering the original definition of $A(M_L M_S)$ given by (7), this function is readily seen to be a partition. In particular, it represents the number of unique ways in which N integers m_i , restricted by $-l \leq m_i \leq l$, can add to give M_L and the number of ways N related quantities $\mu_i = \pm \frac{1}{2}$ can add to give M_S with the added restriction that the simultaneous equalities $m_i = m_j$, $\mu_i = \mu_j$ are disallowed for all $i \neq j$. To relate A to a simpler partition from which a recursion relationship can be obtained, we separate the sets $\{m_i, \mu_i\}$ according to the number of pairs of m_i that are equal (three or more m_i may not be equal).

$$A. m_1 > \dots > m_N$$

The number of states for each given set of m_i satisfying these conditions is the number of unique ways the μ_i can be distributed consistent with $\sum \mu_i = M_S$, which is

$$\binom{N}{\frac{1}{2}N + M_S}. \quad (11)$$

To obtain the total number of states in this category, (11) must be multiplied by the number of unique sets of m_i which satisfy the conditions above, and whose sum is M_L . This number is represented by

$$\sum_{m_1 > \dots > m_N} \delta(\sum m_i, M_L). \quad (12)$$

$$B. m_1 = m_2 \neq \{m_3 > \dots > m_N\}$$

For a given set of m_i satisfying these conditions, one spin-up and one spin-down are necessarily associated with m_1 and m_2 , hence the number of states for each given set of m_i is

$$\binom{N-2}{\frac{1}{2}N-1+M_S}. \quad (13)$$

The total number of states of this kind is therefore the product of (13) with

$$\sum_{m_1=m_2 \neq \{m_3 > \dots > m_N\}} \delta(\sum m_i, M_L). \quad (14)$$

$$C. \{m_1 = m_2 > m_3 = m_4 > \dots > m_{2p-1} = m_{2p}\} \\ \neq \{m_{2p+1} > \dots > m_N\}$$

For this general case, the total number of states is

$$\binom{N-2p}{\frac{1}{2}N-p+M_S} \sum_{\{p\}} \delta(\sum m_i, M_L), \quad (15)$$

where $\{p\}$ represents the lengthy restriction on the m_i given above by C .

The partition A is equal to the summation over all the possibilities for p which is

$$A(M_L M_S) = \sum_{p=0}^{\frac{1}{2}N-1} \binom{N-2p}{\frac{1}{2}N-p+M_S} F(lNM_L p), \quad (16)$$

where F is the partition defined for arbitrary L by,

$$F(lNLp) = \sum_{\{p\}} \delta(\sum m_i, L). \quad (17)$$

This method for expressing A in terms of a new partition F is by no means unique. For example, a given set $\{m_i, \mu_i\}$ can be split into two sets of m_i , those belonging to $\mu_i = +\frac{1}{2}$ and those belonging to $\mu_i = -\frac{1}{2}$. The physical requirements on the m_i now are that no two m_i in the same set are equal, and no reference is made to the equality or inequality of m_i in different sets. A consideration of A from this point of view leads to a new expression for A that can be obtained directly, however this expression will be obtained indirectly but more profitably later in the paper.

III. THE RECURSION RELATIONSHIP

The partition $F(lNLp)$ defined by (17) may be defined alternatively as the number of ways one can choose $N-p$ integers m'_i with the properties that $m'_1 > \dots > m'_{N-p}$, $-l \leq m'_i \leq l$, and that p of these integers are doubled when performing the summation to give L . When viewed in this manner, F readily can be related to itself through a recursion formula. Consider the sets $\{m'_i\}$ that satisfy the conditions for belonging to $F(lNLp)$. These sets can be separated into four categories determined by the two independent possibilities: m'_1 equals or does not equal l , and m'_{N-p} equals or does not equal $-l$. By this explicit consideration of the m'_i that can attain the extremum values $\pm l$, the number of sets of m'_i in each category can be related to F of the form $F(l-1 N' L' p')$. The results are

$$m'_1 \neq l, m'_{N-p} \neq -l: F(l-1 N L p), \quad (18)$$

$$m'_1 = l, m'_{N-p} \neq -l: F(l-1 N-1 L-l p) \\ + F(l-1 N-2 L-2l p-1), \quad (19)$$

$$\begin{aligned}
m'_1 \neq l, m'_{N-p} = -l: & F(l-1 N-1 L+l p) \\
& + F(l-1 N-2 L+2l p-1), \quad (20) \\
m'_1 = l, m'_{N-p} = -l: & F(l-1 N-2 L p) \\
& + F(l-1 N-3 L-l p-1) \\
& + F(l-1 N-3 L+l p-1) \\
& + F(l-1 N-4 L p-2). \quad (21)
\end{aligned}$$

The quantity $F(lNLp)$ is therefore equal to the summation of the nine terms in (18) through (21), since there are no other possibilities for m'_1 and m'_{N-p} .

The recursion relationship for b is obtained by relating F to b through (10) and (16), and using the above recursion formula for F . The result can be expressed in the following symmetric form:

$$\begin{aligned}
b(lNLS) \\
= \sum_{\lambda_1 \dots \lambda_4} \prod_i \binom{1}{\lambda_i} b[l-1, N-2-\lambda_1-\lambda_2+\lambda_3+\lambda_4, \\
L+l(\lambda_1-\lambda_2+\lambda_3-\lambda_4), S + \frac{1}{2}(-\lambda_1+\lambda_2+\lambda_3-\lambda_4)]. \quad (22)
\end{aligned}$$

The physically significant values for b are generated by this recursion formula starting with the following boundary conditions for $l = 0$,

$$b(0000) = 1, b(010\frac{1}{2}) = 1, \quad (23)$$

and the symmetries

$$b(l N - L S) = -b(l N L - 1 S), \quad (24)$$

$$b(l N L - S) = -b(l N L S - 1), \quad (25)$$

$$b(l N L S) = b(l 2(2l+1) - N L S), \quad (26)$$

which can be obtained from (10). It can be further shown that the symmetries will be propagated to all b by the recursion relationship once incorporated into the boundary conditions. Consequently, it is convenient to combine the set of conditions (23) through (26) into the following compact form:

$$\begin{aligned}
b[0 \alpha + \beta - \lambda \frac{1}{2}(\alpha - \beta)] \\
= (-)^{\lambda} \binom{1}{\lambda} \sum_{\sigma} (-)^{\sigma} \binom{1}{\sigma} \binom{1}{\alpha + \sigma} \binom{1}{\beta - \sigma}. \quad (27)
\end{aligned}$$

Expressions (22) and (27) are sufficient to generate all the physically significant b and to ensure the symmetry conditions.

By repeated application of the recursion relationship (22), one can obtain a general solution for $b(lNLS)$ in terms of the boundary values $b(0N'L'S')$. If, then, the solution is specialized to the $b(0N'L'S')$ given by (27), a new, symmetric expression for b

will result which can be recognized as the partition described at the end of Sec. II.

To simplify the calculation, it is convenient first to define two functions, $B_{\lambda}^k(x)$ and $g_{\lambda}^k(\mu)$ as follows:

$$\prod_{r=0}^k (1 + yx^r) = \sum_{\lambda} B_{\lambda}^k(x) y^{\lambda} \quad (28)$$

$$= \sum_{\lambda, \mu} g_{\lambda}^k(\mu) y^{\lambda} x^{\mu}. \quad (29)$$

The difference equations satisfied by these functions are, respectively,

$$B_{\lambda}^k(x) = B_{\lambda}^{k-1}(x) + x^k B_{\lambda-1}^{k-1}(x) \quad (30)$$

and

$$g_{\lambda}^k(\mu) = g_{\lambda}^{k-1}(\mu) + g_{\lambda-1}^{k-1}(\mu), \quad (31)$$

which have the following particular solutions satisfying (28) and (29):

$$B_{\lambda}^k(x) = x^{k\lambda(\lambda-1)} \prod_{r=1}^{\lambda} (1 - x^{k+2-r})(1 - x^r)^{-1} \quad (32)$$

and

$$g_{\lambda}^k(\mu) = \sum_{n_1=0}^k \sum_{n_2=0}^{n_1-1} \dots \sum_{n_{\lambda-1}=0}^{n_{\lambda-2}-1} \delta(\sum n_i, \mu) \quad (33)$$

with

$$B_0^k(x) = 1 \quad (34)$$

and

$$g_0^k(\mu) = \delta_{\mu 0}. \quad (35)$$

The function $g_{\lambda}^k(\mu)$ has, in addition, the following properties that are useful for this problem, and which are easily derived from (29):

$$g_{\lambda}^k(\mu) = g_{\lambda}^k(k\lambda - \mu), \quad (36)$$

$$g_{\lambda}^k(\mu) = g_{k+1-\lambda}^k(\frac{1}{2}k(k+1) - \mu). \quad (37)$$

The iterated application of the recursion relationship (22) results in the expression

$$\begin{aligned}
b(lNLS) \\
= \sum_{\lambda_i, \mu_i} \prod_i g(i) b[0, N-2-\lambda_1-\lambda_2+\lambda_3+\lambda_4, \\
L + \mu_1 - \mu_2 + \mu_3 - \mu_4, S + \frac{1}{2}(-\lambda_1+\lambda_2+\lambda_3-\lambda_4)], \quad (38)
\end{aligned}$$

where the temporary designation $g(i)$ has been given to the expression

$$\begin{aligned}
g(i) = \sum_{\lambda_1 \dots \lambda_{i+1}} \delta(\sum_i \lambda_i, \lambda_i) \delta(\sum_i (l+1-j)\lambda_{ij}, \mu_i) \\
\times \prod_{j=1}^i \binom{1}{\lambda_{ij}}. \quad (39)
\end{aligned}$$

Expressing the Kronecker deltas in (39) by appropriate contour integrals, one obtains

$$g(i) = (2\pi i)^{-2} \oint dy \oint dx y^{-\lambda_i-1} x^{-\mu_i-1} \times \prod_{r=0}^{l-1} (1 + yx^r), \quad (40)$$

which, from (29), is

$$g(i) = g_{\lambda_i}^{l-1}(\mu_i - \lambda_i). \quad (41)$$

The boundary conditions given by (27) can be enforced in the general solution (38) by appropriate Kronecker deltas to give the following special solution:

$$b(lNLS) = \sum_{\alpha\beta\lambda\sigma} (-)^{\lambda+\sigma} \begin{pmatrix} 1 \\ \alpha \end{pmatrix} \begin{pmatrix} 1 \\ \beta \end{pmatrix} \begin{pmatrix} 1 \\ \lambda \end{pmatrix} \begin{pmatrix} 1 \\ \sigma \end{pmatrix} \times \sum_{\lambda_i, \mu_i} \prod_i g_{\lambda_i}^{l-1}(\mu_i - \lambda_i) \times \delta(\tfrac{1}{2}N + S + \sigma - l - \alpha - \lambda_1 + \lambda_3, 0) \times \delta(\tfrac{1}{2}N - S - \sigma - l - \beta - \lambda_2 + \lambda_4, 0) \times \delta(L + \lambda + \mu_1 - \mu_2 + \mu_3 - \mu_4, 0). \quad (42)$$

Owing to the restriction on the arguments of the g , the Kronecker deltas together with these functions can be expressed as three contour integrals in the manner of (40). One obtains the following result:

$$b(lNLS) = \sum_{\lambda\sigma} (-)^{\lambda+\sigma} \begin{pmatrix} 1 \\ \lambda \end{pmatrix} \begin{pmatrix} 1 \\ \sigma \end{pmatrix} (2\pi i)^{-3} \times \oint dx \oint dy \oint dz x^{L+\lambda-1} \times y^{\frac{1}{2}N+S+\sigma-l-2} z^{\frac{1}{2}N-S-\sigma-l-2} (1+y)(1+z) \times \prod_{r=0}^{l-1} (1 + y^{-1}x^{r+1})(1 + yx^{r+1}) \times (1 + z^{-1}x^{-r-1})(1 + zx^{-r-1}), \quad (43)$$

where the summations over α and β have introduced the factors $y^{-1}(1+y)z^{-1}(1+z)$. These are just the factors required to combine the pi products involving y and z separately to obtain

$$(yz)^{-l} \prod_{r=0}^{2l} (1 + yx^{-l}x^r)(1 + zx^l x^{-r}). \quad (44)$$

The contours are then evaluated using (29), and the arguments rearranged according to (36) and (37) to obtain finally,

$$b(lNLS) = \sum_{\lambda\sigma} (-)^{\lambda+\sigma} \begin{pmatrix} 1 \\ \lambda \end{pmatrix} \begin{pmatrix} 1 \\ \sigma \end{pmatrix} \times \sum_{\mu} g_{\frac{1}{2}N+S+\sigma}^{2l}(\mu) g_{\frac{1}{2}N-S-\sigma}^{2l}(Nl+L+\lambda-\mu). \quad (45)$$

Considering the definition of g given by (33), and the alternative method for expressing A according to the discussion at the end of Sec. II, it is clear that the summation over μ in (45) is related to A by

$$A(M_L M_S) = \sum_{\mu} g_{\frac{1}{2}N+M_S}^{2l}(\mu) g_{\frac{1}{2}N-M_S}^{2l}(Nl+M_L-\mu). \quad (46)$$

The somewhat lengthy method employed in the derivation of (45) clarifies the method of obtaining a generating function for the b . By operating on (45) with $\sum_L x^L$ and letting $L = \mu' - Nl - \lambda + \mu$ on the right-hand side, then according to (28) and (29), one has

$$\sum_L b(lNLS)x^L = \sum_{\lambda\sigma} (-)^{\lambda+\sigma} \begin{pmatrix} 1 \\ \lambda \end{pmatrix} \begin{pmatrix} 1 \\ \sigma \end{pmatrix} \times x^{-Nl-\lambda} B_{\frac{1}{2}N+S+\sigma}^{2l}(x) B_{\frac{1}{2}N-S-\sigma}^{2l}(x). \quad (47)$$

The right-hand side of (47) is the generating function of Curl and Kilpatrick, where the explicit values for the B are given by (32).

A more compact generating function is obtained by introducing two new variables by operating on (47) with $\sum_{N_S} y^{\frac{1}{2}N+S} z^{\frac{1}{2}N-S}$. Then we obtain

$$\sum_{L\alpha\beta} b[l\alpha+\beta L \tfrac{1}{2}(\alpha-\beta)] x^L y^{\alpha} z^{\beta} = (1-x^{-1})(1-zy^{-1}) \times \prod_{r=-l}^l (1+yx^r)(1+zx^r), \quad (48)$$

which also can be deduced directly from (43).

With this result, the aims of this paper have been fulfilled. The recursion relationship for the b given by (22) has been most useful for obtaining the values of b in the range $1 \leq l \leq 6$, and these are available on request.⁷ In Tables I, II, and III of this paper the values for $l = 4$ are included to supplement existing tables for $1 \leq l \leq 3$ that appear in several places in the literature.

ACKNOWLEDGMENTS

The author wishes to acknowledge with many thanks the assistance of C. A. Morrison in obtaining and refining several of the results of this paper. He also thanks Arthur Hausner for programming the problem for the HDL computer and for his general interest.