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On the Symmetry of Slater Determinantal Wavefunctions

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A method involving the use of characteristic polynomials of irreducible representation matrices of groups and yielding the symmetry species of Slater determinantal functions is given. The necessary polynomials have been calculated for the commonly occurring symmetry groups and are listed to supplement the usual character tables.

I. INTRODUCTION

THE use of the theory of group representations to simplify quantum-mechanical calculations is so well known as to require no review.¹ Nevertheless, a brief resumé of the steps in a frequently used procedure is useful as a preface to this discussion.

After the group of covering operations for the Hamiltonian has been determined, linear combinations belonging to definite symmetry species are formed from some set of basis functions. Frequently, these are one-electron functions to be used for constructing Slater determinantal functions (SDF) to represent approximate, antisymmetric states of the complete n -electron system. The symmetry species of the determinantal functions can be elucidated in a straightforward manner by calculating the characters and performing the usual species analysis. The determinations of these characters can be quite arduous, however, particularly for excited states of systems having degenerate symmetry species.

This article discusses a fairly simple algorithm which can be used to determine the symmetry species of determinantal functions from the species of the occupied one-electron orbitals. This procedure does not determine the actual linear combinations belonging to each species, but knowing in advance which species projection operators to use can save considerable labor.

II. DERIVATION OF ALGORITHM

A. Spin-Free Case

The system is assumed to have symmetry species $\Gamma_1, \Gamma_2, \Gamma_3, \dots, \Gamma_k$, not necessarily distinct, which are partially or completely filled with electrons in the Slater determinantal function (SDF). The configuration is then $\Gamma_1^{n_1}\Gamma_2^{n_2}\dots\Gamma_k^{n_k}$ with n_i the number of electrons occupying the i th symmetry species. For an SDF of n electrons, we have $n = \sum n_i$. If the degeneracy of Γ_i is g_i and the possibility of both spin orientations is included, the number of linearly independent SDF in the configuration is $G = \prod_i [(2g_i)!/n_i!(2g_i - n_i)!]$, which is, of course, the familiar Fermi-Dirac counting formula. If interest is centered on SDF, specified so

that among the electrons n_i in Γ_i , p_i have m_S values of $+\frac{1}{2}$ and $n_i - p_i$ have m_S values of $-\frac{1}{2}$, the total M_S value is then $(\frac{1}{2}) \sum_i (2p_i - n_i)$. The number of linearly independent SDF in the configuration of this type is

$$G(p) = \prod_i \left[\frac{g_i!}{p_i!(g_i - p_i)!} \frac{g_i!}{(n_i - p_i)!(g_i + p_i - n_i)!} \right]$$

If one of the $G(p)$ SDF is subjected to transformation by \mathcal{R} , one of the covering operations of the group, a linear combination of the SDF is obtained. If the \mathcal{R} are assumed to be spin free, M_S is unchanged in the process. If $\Psi(p)$ denotes the subset designated by p_i of all the SDF belonging to the configuration, $\Psi(p) \rightarrow \mathcal{R}\Psi(p)$ is a linear transformation represented by a $G(p) \times G(p)$ matrix. The trace (character) of the matrix is needed.

In order to calculate the trace, the effect of \mathcal{R} on one of the symmetry species is determined. The p_i spin orbitals from Γ_i with $m_S = \frac{1}{2}$ are transformed among themselves by \mathcal{R} , since these functions are assumed to form a basis for an irreducible representation of the group. The spin orbitals are denoted $u_i(j)\alpha$, $j = 1, 2, \dots, g_i$. p_i of these are involved in any one SDF. Thus, one obtains

$$\mathcal{R}u_i(j)\alpha = \sum_k D_i(\mathcal{R})_{kj} u_i(k)\alpha.$$

If the SDF contains $u_i(j_1)\alpha$, $u_i(j_2)\alpha$, \dots , $u_i(j_{p_i})\alpha$ and similarly $u_i(k_1)\beta$, $u_i(k_2)\beta$, \dots , $u_i(k_{n_i - p_i})\beta$, the diagonal element of the matrix giving the linear transformation $\mathcal{R}\Psi(p)$ is a product of determinants obtained from the irreducible-representation matrices $D_i(\mathcal{R})$. From Γ_i we obtain the product of two determinants: one is the $p_i \times p_i$ determinant constructed from the j_1 row and column, j_2 row and column, \dots , j_{p_i} row and column of $D_i(\mathcal{R})$. The other determinant is the similarly constructed one from the $m_S = -\frac{1}{2}$ functions with $n_i - p_i$ rows and columns. If we sum over the $[g_i! / p_i!(g_i - p_i)!]$ diagonal elements of the linear transformation $\mathcal{R}\Psi(p)$ corresponding to all the possible ways that the $u_i(j)\alpha$ may be occupied, it is easily seen that the contribution from Γ_i , $m_S = +\frac{1}{2}$ states is just $(-1)^{q_i - p_i}$ times the coefficient of $\mu^{q_i - p_i}$ in the characteristic polynomial for $D_i(\mathcal{R})$:

$$Q_i(\mathcal{R}, \mu) = |D_i(\mathcal{R}) - \mu I|.$$

¹ (a) E. P. Wigner, *Group Theory* (Academic Press Inc., New York, 1959); (b) H. Eyring, J. Walter, and G. E. Kimball, *Quantum Chemistry* (John Wiley & Sons, Inc., New York, 1944).

It is more convenient below to have the polynomials arranged so that the exponent corresponds to the number of electrons rather than the g_i complement and to have the signs all positive, therefore a new indeterminate $\lambda = 1/\mu$ is introduced and Q_i is transformed:

$$P_i(\mathcal{R}, \lambda) = \lambda^{g_i} Q_i(\mathcal{R}, -1/\lambda) = |\lambda D_i(\mathcal{R}) + I|.$$

Since the characteristic polynomial depends only upon the eigenvalues of a matrix, and each group-representation element belonging to a given class has the same eigenvalues, $P_i(\mathcal{R}, \lambda)$ will be a class function of the group. The coefficients of a given power of λ in all of the $P_i(\mathcal{R}, \lambda)$ form a character of a reducible or irreducible representation of the group, so the results could be summarized by giving one polynomial with the coefficient of λ^i written as the appropriate symmetry species (irreducible representation) or sum of symmetry species. The argument \mathcal{R} may now be suppressed from the symbol $P_i(\mathcal{R}, \lambda)$.

Once the $P_i(\lambda)$ have been determined for each occupied symmetry species of the SDF, the composite symmetry is easily determined by forming the product

$$P = \prod_{i=1}^k P_i(\lambda_i) P_i(\lambda_i'),$$

where species multiplication as determined by the group is used to evaluate the new coefficients. The coefficient of $\lambda_1^{p_1} (\lambda_1')^{n_1 - p_1} \lambda_2^{p_2} (\lambda_2')^{n_2 - p_2} \dots$ in P gives the symmetry species contained in the original SDF.

In general discussions of the theory of group representations^{1b} it is customary to collect together a number of results in the form of character tables. Such collections do not usually contain the characteristic polynomials of the irreducible representation matrices. Therefore, the $P_i(\lambda)$ are given in Appendix A for the degenerate representations of the point groups commonly given in such listings. The one dimensional representations can be obtained immediately, since in this case the character and the eigenvalue are the same.

B. Generalization to Include Spin

The foregoing discussion would not give particularly useful results unless it could be generalized to include the computation of the correct spin states. This is easily done by calculating the characteristic polynomials associated with the product group formed from the point group appropriate for the space part of the spin orbitals and the two-dimensional unimodular, unitary group appropriate for the spin functions. This is easily done by examining the eigenvalues of a group element in each class. Again the results may be summarized by giving a single polynomial with the species notation given for each coefficient. The spin states are given by the usual anterior superscript $2S+1$. If these new polynomials are denoted $R_i(\lambda)$, the correct symmetry and spin states are given by the coefficient of

$\lambda_1^{n_1} \lambda_2^{n_2} \lambda_3^{n_3} \dots$ in the product

$$R = \prod_{i=1}^k R_i(\lambda_i),$$

where we have obtained $R_i(\lambda)$ from the characteristic polynomial by a transformation similar to $Q_i \rightarrow P_i$. Again, the coefficients in R are computed from the species product rules of the group of the space functions and the standard decomposition formula for angular momentum,

$$(2S+1) \times (2S'+1) \\ = [2(S+S'+1), [2(S+S')-1], \dots, \\ [2|S-S'|+1].$$

The polynomials $R_i(\lambda)$ are also given in Appendix A for the degenerate species of the common point groups. The foregoing discussion applies equally well to both continuous and discrete groups and Appendix B gives a method of generating the $R_i(\lambda)$ for the atomic case of Russel-Saunders coupling.

III. EXAMPLES

Although the foregoing discussion is fairly self-explanatory, examples might be useful to clarify the procedure. We consider the following cases.

A. Some Excited States of Benzene, D_{6h}

If the Hückel molecular orbitals for the π system of benzene have been determined in the standard fashion, the symmetry species of the one-electron functions are $A_{2u}, E_{1g}, E_{2u}, B_{2g}$.² The configurations $A_{2u}^2 E_{1g}^{4-i} E_{2u}^i$, $i=0, 1, 2, 3, 4$ may be obtained by examining the product of the R polynomials corresponding to the A_{2u}, E_{1g} , and E_{2u} species. We get from Table IV in Appendix A

$$\begin{aligned} & [{}^1A_{1g}(\lambda_1^2+1) + {}^2A_{2u}\lambda_1] [{}^1A_{1g}(\lambda_2^4+1) + {}^2E_{1g}(\lambda_2^3+\lambda_2) \\ & + ({}^3A_{2g} + {}^1A_{1g} + {}^1E_{2g})\lambda_2^2] [{}^1A_{1g}(\lambda_3^4+1) + {}^2E_{2u}(\lambda_3^3+\lambda_3) \\ & + ({}^3A_{2g} + {}^1A_{1g} + {}^1E_{2g})\lambda_3^2] = {}^1A_{1g}(\lambda_1^2\lambda_2^4 + \lambda_1^2\lambda_3^4) \\ & + ({}^3B_{1u} + {}^3B_{2u} + {}^3E_{1u} + {}^1B_{1u} + {}^1B_{2u} + {}^1E_{1u}) \\ & \times (\lambda_1^2\lambda_2^3\lambda_3 + \lambda_1^2\lambda_2\lambda_3^3) + ({}^5A_{1g} + {}^3A_{1g} + {}^2^3A_{2g} \\ & + {}^2^3E_{2g} + {}^3^1A_{1g} + {}^1A_{2g} + {}^3^1E_{2g})\lambda_1^2\lambda_2^3\lambda_3^2 \\ & + (\text{terms with sum of exponents} \neq 6). \end{aligned}$$

The coefficient of $\lambda_1^2\lambda_2^4\lambda_3^i$ gives the states present in the configurations. The terms in the polynomial not given correspond to configurations of ionized benzene.

B. Atomic Configuration d^2

From Table VII in Appendix B we find that the characteristic polynomial for equivalent d (which are

² G. W. King, *Spectroscopy and Molecular Structure* (Holt, Rinehart and Winston, Inc., New York, 1964).

TABLE I. Polynomials P for two-dimensional representations of common, finite point groups and $C_{\infty v}$ and $D_{\infty h}$.

Group	Species	λ^2	λ	λ^0
D_3, C_{3v}	E	A_2	E	A_1
D_4, C_{4v}	E	A_2	E	A_1
D_6, C_{6v}	E_i	A_2	E_i	A_1
D_6, C_{6v}	E_i	A_2	E_i	A_1
D_{3h}	$E^{(p)}$	A_2'	$E^{(p)}$	A_1'
D_{4h}	$E_{g(u)}$	A_{2g}	$E_{g(u)}$	A_{1g}
D_{6h}	$E_i^{(p)}$	A_2'	$E_i^{(p)}$	A_1'
D_{6h}	$E_{ig(u)}$	A_{2g}	$E_{ig(u)}$	A_{1g}
D_{2d}	E	A_2	E	A_1
D_{3d}	$E_{g(u)}$	A_{2g}	$E_{g(u)}$	A_{1g}
D_{4d}	E_i	A_2	E_i	A_1
D_{6d}	$E_{ig(u)}$	A_{2g}	$E_{ig(u)}$	A_{1g}
D_{6d}	E_i	A_2	E_i	A_1
T_d, O	E	A_2	E	A_1
O_h	$E_{g(u)}$	A_{2g}	$E_{g(u)}$	A_{1g}
$C_{\infty v}$	Λ	Σ^-	Λ	Σ^+
$D_{\infty h}$	$\Lambda_{g(u)}$	Σ_g^-	$\Lambda_{g(u)}$	Σ_g^+

* Λ stands for Π, Δ, Φ , etc.

even) electrons is given by

$$G_0^e G_1^e G_2^e = [^1S^e(\lambda^2+1) + ^2S^e\lambda][^1S^e(\lambda^4+1) + (^2P^e - ^2S^e)(\lambda^3+\lambda) + (^3S^e + ^1S^e + ^1D^e - ^1P^e)\lambda^2][^1S^e(\lambda^4+1) + (^2D^e - ^2P^e)(\lambda^3+\lambda) + (^3S^e + ^1S^e + ^1G^e - ^1F^e)\lambda^2].$$

The coefficient of λ^2 (and λ^8) in this polynomial is

$$^1S^e + ^1G^e + ^3F^e + ^3P^e + ^1D^e.$$

This result is very familiar, of course, being obtainable by several other methods.

APPENDIX A

This appendix collects the results (Tables I-VI) for the Polynomials P_i and R_i for the degenerate species of the common groups. As was mentioned above, P_i and R_i may be written down by inspection for one-dimensional species. Thus, if X is the species notation for any one-dimensional species of any group and A the symbol

TABLE II. Polynomials P for three-dimensional representations of Point Groups $T, T_d, O_h, I,$ and I_h .

Group	Species	λ^3	λ^2	λ	λ^0
T	F	A	F	F	A
T_h	$F_{g(u)}$	$A_{g(u)}$	F_g	$F_{g(u)}$	A_g
T_d, O	F_i	A_i	F_1	F_i	A_1
O_h	$F_{ig(u)}$	$A_{ig(u)}$	F_{1g}	$F_{ig(u)}$	A_{1g}
I	F_i	A	F_i	F_i	A
I_h	$F_{ig(u)}$	$A_{g(u)}$	F_{ig}	$F_{ig(u)}$	A_g

for the totally symmetric species,

$$P = X\lambda + A$$

and

$$R = ^1A(\lambda^2+1) + ^2X\lambda.$$

APPENDIX B

Herein is given a method for obtaining R polynomials for the product group of the three-dimensional rotation group R_3 with the two-dimensional unimodular unitary group U_2 for application to Russell-Saunders states for atomic configurations. The fact that these groups are homomorphic does not enter into the present calculations. The method is given in some detail since a simple modification was used to obtain the results listed in Appendix A.

A class of R_3 or U_2 consists of all rotations by a given angle about any axis. The character of the j th irreducible representation is $[\sin(j+\frac{1}{2})\theta/\sin\theta/2]$ where j

TABLE III. Polynomials P for four- and five-dimensional representations of I and I_h .

$I:$	$G:$	$A\lambda^4 + G\lambda^2 + (F_1 + F_2)\lambda^2 + G\lambda + A$
	$H:$	$A\lambda^6 + H\lambda^4 + (F_1 + F_2 + G)(\lambda^3 + \lambda^2) + H\lambda + A$
$I_h:$	$G_{g(u)}:$	$A_g\lambda^4 + G_{g(u)}\lambda^2 + (F_{1g} + F_{2g})\lambda^2 + G_{g(u)}\lambda + A_g$
	$H_{g(u)}:$	$A_{g(u)}\lambda^6 + H_{g(u)}\lambda^4 + (F_{1g(u)} + F_{2g(u)} + G_{g(u)})\lambda^3 + (F_{1g} + F_{2g} + G_g)\lambda + H_{g(u)}\tau + A_g$

is integral for R_3 and integral or half-integral for U_2 . The actual angle of rotation is θ . The eigenvalues of any unimodular unitary irreducible representation matrix $D(j, \theta)$ in the class θ are $\exp(ij\theta), \exp[i(j-1)\theta], \dots, \exp(-ij\theta)$.³ The irreducible representation matrices for $U_2 \times R_3$ are $D_u(S, \theta) \times D_R(l, \theta')$ and the eigenvalues of this are the products of the eigenvalues of D_u and D_R taken in all combinations. If we set $\xi = \exp(i\theta)$ and $\eta = \exp(i\theta')$, these eigenvalues are $\xi^k \eta^m$ where $k = s, s-1, \dots, -s$ and $m = l, l-1, \dots, -l$. Hence the R polynomial for this representation matrix is

$$R(s, l) = \prod_k \prod_m (\lambda \xi^k \eta^m + 1).$$

It is convenient to change the notation to conform with that commonly used in the theory of atoms. Thus, $D_u(s, \theta) \times D_R(l, \theta')$ can be denoted ^{2s+1}l , $l = S, P, D$, etc. in the standard fashion. Since among the one-electron spin orbitals $S = \frac{1}{2}$, we are actually interested only in the polynomial $R(\frac{1}{2}, l)$. It is ob-

³ F. D. Murnaghan, *The Theory of Group Representations* (The Johns Hopkins Press, Baltimore, Md., 1938).

TABLE IV. Polynomials R for two-dimensional representations of common point groups.

Group	Species	(λ^4+1)	$(\lambda^3+\lambda)$	λ^2
D_3, C_{3v}	E	1A_1	2E	${}^3A_2+{}^1A_1+{}^1E$
D_4, C_{4v}	E	1A_1	2E	${}^3A_2+{}^1A_1+{}^1B_1+{}^1B_2$
D_6, C_{3v}	E_1	1A_1	2E_1	${}^3A_2+{}^1A_1+{}^1E_2$
	E_2	1A_1	3E_2	${}^3A_2+{}^1A_1+{}^1E_1$
D_6, C_{6v}	E_i	1A_1	2E_i	${}^3A_2+{}^1A_1, +{}^1E_2$
D_{3h}	$E^{(p)}$	${}^1A_1'$	${}^2E^{(p)}$	${}^3A_2'+{}^1A_1'+{}^1E'$
D_{4h}	$E_{g(u)}$	${}^1A_{1g}$	${}^2E_{g(u)}$	${}^3A_{2g}+{}^1A_{1g}+{}^1B_{1g}+{}^1B_{2g}$
D_{3h}	$E_1^{(p)}$	${}^1A_1'$	${}^2E_1^{(p)}$	${}^3A_2'+{}^1A_1'+{}^1E_2'$
	$E_2^{(p)}$	${}^1A_1'$	${}^2E_2^{(p)}$	${}^3A_2'+{}^1A_1'+{}^1E_1'$
D_{6h}	$E_{ig(u)}$	${}^1A_{1g}$	${}^2E_{ig(u)}$	${}^3A_{2g}+{}^1A_{1g}+{}^1E_{2g}$
D_{2d}	E	1A_1	2E	${}^3A_2+{}^1A_1+{}^1B_1+{}^1B_2$
D_{3d}	$E_{g(u)}$	${}^1A_{1g}$	${}^2E_{g(u)}$	${}^3A_{2g}+{}^1A_{1g}+{}^1E_g$
D_{4d}	$E_i (i=1, 3)$	1A_1	2E_i	${}^3A_2+{}^1A_1+{}^2E$
	E_2	1A_1	3E_2	${}^3A_2+{}^1A_1+{}^1B_1+{}^1B_2$
D_{6d}	$E_{1g(u)}$	${}^1A_{1g}$	${}^2E_{1g(u)}$	${}^3A_{2g}+{}^1A_{1g}+{}^1E_{2g}$
	$E_{2g(u)}$	${}^1A_{1g}$	${}^2E_{2g(u)}$	${}^3A_{2g}+{}^1A_{1g}+{}^1E_{1g}$
D_{6d}	$E_i (i=1, 5)$	1A_1	2E_i	${}^3A_2+{}^1A_1+{}^1E_2$
	$E_i (i=2, 4)$	1A_1	2E_i	${}^3A_2+{}^1A_1+{}^1E_4$
	E_3	1A_1	2E_3	${}^3A_2+{}^1A_1+{}^1B_1+{}^1B_2$
T_d, O	E	1A_1	2E	${}^3A_2+{}^1A_1+{}^1E$
O_h	$E_{g(u)}$	${}^1A_{1g}$	${}^2E_{g(u)}$	${}^3A_{2g}+{}^1A_{1g}+{}^1E_g$
$C_{\infty v}$	Λ	${}^1\Sigma^+$	${}^2\Lambda$	${}^3\Sigma^-+{}^1\Sigma^++{}^1(2\Lambda)$
$D_{\infty h}$	$\Lambda_{g(u)}$	${}^1\Sigma_g^+$	${}^2\Lambda_{g(u)}$	${}^3\Sigma_g^-+{}^1\Sigma_g^++{}^1(2\Lambda)_g$

TABLE V. Polynomials R for the three-dimensional representations of $T, T_d, T_h, O, O_h, I,$ and I_h .

Group	Species	(λ^6+1)	$(\lambda^6+\lambda)$	$(\lambda^4+\lambda^2)$	λ^3
T	F	1A	2F	${}^3F+2'F$	$4A+2^2F+{}^2E$
T_h	$F_{g(u)}$	1A_g	${}^2F_{g(u)}$	${}^3F_g+2^1F_g$	$4A_{g(u)}+2^2F_{g(u)}+{}^2E_{g(u)}$
T_d, O	F_i	1A_1	2F_i	${}^3F_1+{}^1A_1+{}^1E+{}^1F_2$	${}^4A_i+{}^2E+{}^2F_1+{}^2F_2$
O_h	$F_{ig(u)}$	${}^1A_{1g}$	${}^2F_{ig(u)}$	${}^3F_{ig}+{}^1A_{1g}+{}^1E_g+{}^1F_{2g}$	${}^4A_{ig(u)}+{}^2E_{g(u)}+{}^2F_{ig(u)}+{}^2F_{2g(u)}$
I	F_i	1A	2F_i	${}^3F_i+{}^1A+{}^1H$	${}^4A+{}^2F_i+{}^2H$
I_h	$F_{ig(u)}$	1A_g	${}^2F_{ig(u)}$	${}^3F_{ig}+{}^1A_g+{}^1H_g$	${}^4A_{g(u)}+{}^2F_{ig(u)}+{}^2H_{g(u)}$

TABLE VI. Polynomials R for four- and five-dimensional representations of I and I_h .

I	$G: \quad {}^1A(\lambda_1+1) + {}^2G(\lambda^7+\lambda) + ({}^3F_1+{}^3F_2+{}^1A+{}^1G+{}^1H)(\lambda^6+\lambda^2) + ({}^4G+{}^2P_1+{}^2F_2+{}^2G+{}^2H)(\lambda^5+\lambda^3) + ({}^5A+{}^3F_1+{}^3F_2+{}^3G+{}^3H+{}^1A+{}^1G+{}^3H)\lambda^4$
	$H: \quad {}^1A(\lambda^{10}+1) + {}^2H(\lambda^9+\lambda) + ({}^3F_1+{}^3F_2+{}^3G+{}^1A+{}^1G+{}^2H)(\lambda^8+\lambda^2) + ({}^4F_1+{}^4F_2+{}^4G+{}^2F_1+{}^2F_2+{}^2G+{}^4H)(\lambda^7+\lambda^3) + ({}^5H+{}^3F_1+{}^3F_2+{}^3G+{}^3H+{}^3A+{}^1F_1+{}^1F_2+{}^4G+{}^4H)(\lambda^6+\lambda^4) + ({}^6A+{}^4F_1+{}^4F_2+{}^2G+{}^2H+{}^2A+{}^3F_1+{}^3F_2+{}^5G+{}^7H)\lambda^5$
I_h	Same as I except adding subscript g to all coefficients of even powers of λ and subscript $g(u)$ to coefficients of odd powers of λ for $g(u)$ representations

served that

$$\begin{aligned} & [R(\frac{1}{2}, l+1)/R(\frac{1}{2}, l)] \\ & \equiv G_{l+1}(\lambda) \\ & = (\lambda^4+1) + (\xi^{\frac{1}{2}} + \xi^{-\frac{1}{2}})(\eta^{l+1} + \eta^{-l-1})(\lambda^3 + \lambda) \\ & \quad + [(\xi+1 + \xi^{-1}) + 1 + \eta^{2l+2} + \eta^{-2l-2}]\lambda^2. \end{aligned}$$

It is easily seen that $G_0(\lambda) = (\lambda^2+1) + (\xi^{\frac{1}{2}} + \xi^{-\frac{1}{2}})\lambda$; hence,

we may write

$$R(\frac{1}{2}, l) = \prod_{k=0}^l G_k(\lambda).$$

It is observed that G_l may also be written as

$$\begin{aligned} G_l = & {}^1S(\lambda^4+1) + [{}^2(l) - {}^2(l-1)](\lambda^3 + \lambda) \\ & + [{}^3S+{}^1S+{}^1(2l) - {}^1(2l-1)]\lambda^2. \end{aligned}$$

TABLE VII. The polynomials $G_l(\lambda)$ for atomic states.

$G_0^{(e)} = {}^1S^e(\lambda^2+1) + {}^2S^e\lambda$
$G_1^{(0,e)} = {}^1S^e(\lambda^4+1) + ({}^2D^{(0,e)} - {}^2S^{(0,e)})(\lambda^3 + \lambda) + ({}^3S^e + {}^1S^e + {}^1D^e - {}^1P^e)\lambda^2$
$G_2^{(0,e)} = {}^1S^e(\lambda^4+1) + ({}^2D^{(0,e)} - {}^2P^{(0,e)})(\lambda^3 + \lambda) + ({}^3S^e + {}^1S^e + {}^1G^e - {}^1F^e)\lambda^2$
$G_3^{(0,e)} = {}^1S^e(\lambda^4+1) + ({}^2F^{(0,e)} - {}^2D^{(0,e)})(\lambda^3 + \lambda) + ({}^3S^e + {}^1S^e + {}^1K^e - {}^1H^e)\lambda^2$

If we had used the three-dimensional real orthogonal group O_3 instead of R_3 , the irreducible representations can be classified as odd or even, and since the space part of the individual spin orbitals is odd or even with l , this may be included in the calculation easily. Table VII gives the first few G polynomials in terms of Russell-Saunders term symbols. It may be pointed out that a simple necessary condition for the correctness of the results is the disappearance of all minus signs in R in spite of their presence in the G_l .