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An Automatic Procedure for the Symmetry Blocking of Semi-Empirical Hamiltonians

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We present a procedure for the block-diagonalisation of a Fock matrix which does not require explicit details of the point group of the molecule concerned. The method consists of two parts: (a) the trial eigenvectors determined at the start of a semi-empirical calculation are analysed to give an initial set of symmetry-adapted functions; and (b) these symmetry-adapted functions are modified by testing for a correct blocking in the initial diagonalisation of the Fock matrix. Only minor modifications to existing semi-empirical programs are needed for the inclusion of the routines to perform the algorithm.

1. INTRODUCTION

The value of making explicit consideration of symmetry in molecular orbital calculations has been appreciated for some time. For example in ab initio calculations symmetry can greatly reduce the time associated with evaluating and manipulating n^4 two-electron repulsion integrals [1]. In the semi-empirical methods, such as CNDO, INDO and MINDO, the zero-differential overlap approximation essentially removes the integral problem and now the major part of the calculation involves solving a secular equation [2]. The time required for the eigenvalue problem can be reduced if the Hamiltonian is transformed into block-diagonal form using symmetry-adapted basis functions. Unfortunately, the derivation of suitable symmetry-adapted functions is often difficult and tedious requiring detailed knowledge of the symmetry properties of the relevant point group.

We present here a simple method for generating symmetry-adapted functions suitable for block-diagonalising the Hamiltonian which requires no prior knowledge of the group we are dealing with. Apart from the obvious advantage of performing quicker diagonalisations, we also have two other motives for using a block-diagonalisation approach. Much of our recent work has been with systems involving transition metals and because of the weakly interacting *d*-orbitals, molecular orbitals belonging to different irreducible representations are often almost degenerate. The near accidental degeneracy introduces small rounding errors in the density matrix, which after several SCF iterations cause a breaking of the molecular orbital symmetry. Whilst such molecular orbitals are important in their own right, the block-

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diagonalisation of the Fock matrix ensures that the molecular orbitals retain the features of a particular irreducible representation. Secondly, and again because of the *d*-orbitals, we have found for transition metal systems, several total electronic wavefunctions, which differ in symmetry type, that are close in energy. By identifying the irreducible representation to which an occupied molecular orbital belongs, we can ensure that the total wavefunction always corresponds to a certain configuration [3].

The method consists of two parts: (a) an initial set of symmetry-adapted functions are determined from an analysis of the trial eigenvectors obtained from a Hückel type calculation, and thus these eigenvectors are usually used in forming a "guess" at the density matrix; and (b) the symmetry-adapted functions are refined by checking their ability to correctly block-diagonalise the semi-empirical Fock matrix. The refinement of the symmetry-adapted functions, part (b), is possible because the Fock matrix, which includes the electron–electron interaction terms which were previously absent, does not commute with the Hückel Hamiltonian. We shall see that the method requires little calculation of new information.

A similar procedure for finding the symmetry-adapted functions has been proposed previously by Bouman *et al.* [4, 5] and Chung and Goodman [6] where they analyze the characteristic equations associated with the overlap and kinetic energy matrices. Our method differs in that we identify the equivalent atom sets in the molecule (i.e., the set of atoms which transform into each other through the symmetry operations of the group); this enables the symmetry-adapted functions to span only the atomic orbitals on the equivalent atoms. Secondly, we initially distinguish the irreducible representations by consideration of the orthogonality of the Hückel eigenvectors. An alternative algorithm developed by Bagus and Wahlgren [7] obtains symmetry-adapted functions of the full point group from basis functions and integrals belonging to a subgroup. Their method makes an initial identification of the high symmetry functions by comparing one-electron eigenvalues of the low symmetry blocks. The complete separation of the high symmetry function is effected by using the fact that the kinetic energy and nuclear attraction operators do not commute. The Bagus and Wahlgren algorithm is primarily of value in non-empirical calculation packages. Our method is more applicable to semi-empirical procedures where one only considers the valence molecular orbitals, and where one does not have to be concerned with evaluating n^4 two-electron integrals. The method presented herein has an additional advantage for semi-empirical calculations in that previous methods [4–6] require calculation of the kinetic energy or other special matrices which are not part of semi-empirical procedures whereas this method requires only matrix elements already present.

2. THEORY

2.1. *Basis Set Expansions for Molecular Orbitals*

In the electronic structure calculations of the nature we are interested in here, the complete set of molecular orbitals (MOs) $\{\psi_i\}$ are written as

$$\boldsymbol{\psi} = \boldsymbol{\phi}\mathbf{C}, \tag{1}$$

where

$$\boldsymbol{\psi} = (\psi_1 \psi_2 \cdots), \tag{2}$$

$$\boldsymbol{\phi} = (\phi_1 \phi_2 \cdots) \tag{3}$$

is the appropriate basis set, and

$$\mathbf{C} = (\mathbf{C}_1 \mathbf{C}_2 \cdots) \tag{4}$$

with each eigenvector given as

$$\mathbf{C}_i = \begin{pmatrix} c_{1i} \\ c_{2i} \\ \vdots \end{pmatrix}. \tag{5}$$

In the semi-empirical procedures, such as CNDO, INDO and MINDO, the zero-differential overlap approximation enables the Hartree–Fock–Roothaan eigenvalue equation to be written as

$$\mathbf{HC} = \mathbf{CE}, \tag{6}$$

where $\mathbf{H}$ is some Hamiltonian or Fock matrix and $\mathbf{E}$ is the eigenvalue matrix.

The expansion of the MOs is not unique, one can always expand ψ_i in terms of a different set of basis functions, e.g.,

$$\psi_i = \boldsymbol{\chi} \cdot \mathbf{D}_i \tag{7}$$

where $\{\chi_\lambda\}$ could be some symmetry-adapted functions. The different basis sets can be interrelated through

$$\boldsymbol{\chi} = \boldsymbol{\phi} \cdot \mathbf{T}. \tag{8}$$

The symmetry of the Hamiltonian H will require the MOs ψ_i to have the same transformation properties as an irreducible representation of the point group involved. Similarly, one can choose the basis functions χ_μ to transform as irreducible representations; such a basis function is generally called "symmetry-adapted." In our algorithm we require that $\{\chi_\mu\}$ have the following properties:

(1) χ_μ must be composed of atomic orbitals all with the same l value. The symmetry operations do not mix orbitals with different l values, e.g., p_x and p_y may be mixed after some operations but s and p will always be separate.

(2) χ_μ must consist of atomic orbitals belonging to the same equivalent atom set. This is not an essential condition but does reduce the size of the transformations involved in block-diagonalising the Fock matrix.

(3) For degenerate MOs, all the χ_μ's must be in phase. By being in phase we mean that $d_{\mu i}$ is the same for degenerate components of ψ_i.

From the above three properties, one can expand the g-fold degenerate MO belonging to the Rth irreducible representation as

$$\psi_i^{R,\alpha} = \sum_l \sum_a \sum_\lambda \chi_{la}^{R,\lambda\alpha} d_{la,i}^{R,\lambda}, \qquad \alpha = 1,\ldots, g, \tag{9}$$

where l sums over the atomic orbital types, a over the different equivalent atom sets, λ allows for more than one χ with the same la index and α labels the different degenerate components. The summations in (9) only include the functions which belong to the Rth irreducible representation.

We should also note that $\mathbf{C}$ and $\mathbf{D}$ can be related, substituting Eq. (8) into (7) and comparing with Eq. (1) gives

$$\mathbf{C}_i^{R,\alpha} = \mathbf{T}^{R,\alpha} \cdot \mathbf{D}_i^R, \qquad \alpha = 1,\ldots, g, \tag{10}$$

where $\mathbf{T}^{R,\alpha}$ is the transformation matrix for the Rth irreducible representation.

It is through Eqs. (9) and (10) that we obtain a set of symmetry functions suitable for block-diagonalising the Fock matrix. In the next section we give the details of our algorithm for choosing the symmetry-adapted functions.

2.2. *Generation of Symmetric Basis Sets*

This section is broken into two parts were we describe:

(a) the initial search for symmetry-adapted functions; and

(b) the refinement of the symmetry-adapted functions so as to ensure the Fock matrix is correctly block-diagonalised.

2.2a. *Initial Symmetry Function Search*

The equivalent atom sets are first identified by checking the density matrix

$$P_{\mu\nu} = \sum_i^{\text{occ}} c_{\mu i} c_{\nu i}. \tag{11}$$

Those atoms which are equivalent to each other will have the sum of the diagonal $P_{\mu\nu}$ matrix elements for a particular orbital type the same, e.g., for the p-orbitals

$$P_p^A = \sum_{\mu \text{ on atom } A}^{l=1} P_{\mu\mu}. \tag{12}$$

In the program we treat those atoms which have matching P_s^A, P_p^A and P_d^A as forming an equivalent set.

After obtaining the equivalent atom sets we start the decomposition of the eigenvectors. From the requirements of the symmetry-adapted functions χ_μ given in Section 2.1, let us write the molecular orbital we are dealing with as

$$\begin{aligned}\psi_i^\alpha &= \sum_l \sum_a \theta_{la}^\alpha h_{la,i} \\ &= \sum_L \theta_L^\alpha h_{L,i}, \qquad \alpha = 1,\ldots, g,\end{aligned} \tag{13}$$

where L is the combined l and a indices; the θ_L^α are given by

$$\theta_L^\alpha = \sum_{\mu(l\text{ type, } a\text{ unique atom set})} \phi_\mu U_{\mu,L}^\alpha \tag{14}$$

and represent normalised components of the molecular orbital belonging to the lth orbital type of the ath equivalent atom set. That is, the program decomposes the eigenvectors $\mathbf{C}_i^\alpha$ into vectors spanning different l types and equivalent atom sets and renormalises these components to give $\mathbf{U}_L^\alpha$. These $\mathbf{U}_L^\alpha$ are the vectors from which the symmetry-adapted functions are obtained. The molecular orbitals are taken to be degenerate when the related eigenvalues obey

$$|\varepsilon_i - \varepsilon_{i+1}| < \text{Threshold}, \tag{15}$$

where in practice thresholds of 10^{-8} have been used. Some accidental degeneracies amongst the valence molecular orbitals may occasionally occur, however, these usually can be removed by modifying the atomic orbital overlap.

If ψ_i^α is the first molecular orbital of its degeneracy to be examined, then the $\mathbf{U}_L^\alpha$ is taken as the first symmetry function, i.e.,

$$\chi_L^{1,1\alpha} = \theta_L^\alpha, \qquad \alpha = 1,\ldots, g \tag{16}$$

or

$$\mathbf{T}_L^{1,1\alpha} = \mathbf{U}_L^\alpha, \qquad \alpha = 1,\ldots, g. \tag{17}$$

When ψ_i^α is not the first molecular orbital of its degeneracy, the square of the scalar product

$$\begin{aligned}S_L^R &= \sum_\alpha \sum_\beta \sum_\lambda^{\lambda_{\max}} (\chi_L^{R,\lambda\alpha}, \theta_L^\beta)^2 \\ &= \sum_\alpha \sum_\beta \sum_\lambda^{\lambda_{\max}} \{(\mathbf{T}_L^{R,\lambda\alpha})^T \cdot \mathbf{U}_L^\beta\}^2\end{aligned} \tag{18}$$

is evaluated, where $\lambda_{\max}$ is the maximum number of χ for a particular irreducible representation R with L index determined so far. We should also recall that group theory requires the orthogonality condition

$$(\chi_L^{R,\lambda\alpha}, \chi_{L'}^{R',\lambda'\alpha'}) = \delta_{RR'}\delta_{\lambda\lambda'}\delta_{\alpha\alpha'}\delta_{LL'}, \tag{19}$$

where we also assume that the symmetry-adapted functions are normalised.

Now consider the case of a non-degenerate molecular orbital, and assume that we have already several χ belonging to p different irreducible representations. The decomposed functions θ can be expanded as a linear combination of the symmetry-adapted functions, namely,

$$\theta_L^1 = \sum_{\lambda} a_\lambda \chi_L^{Q,\lambda 1} \tag{20}$$

and thus the scalar product S_L^R can have three types of values:

$$\text{(i)} \qquad S_L^R = 1, \tag{21a}$$

$$\text{(ii)} \qquad S_L^R = 0, \tag{21b}$$

$$\text{(iii)} \qquad 0 < S_L^R < 1. \tag{21c}$$

Situation (i) indicates that θ_L^1 is a linear combination, spanning completely all the symmetry functions χ with L index in the Rth irreducible representation and nothing further needs to be done with θ_L^1.

When S_L^R is zero, this indicates that θ_L^1 is orthogonal to the symmetry functions of Rth irreducible representation. If all of the θ_L^1 give zero scalar products with each of the known symmetry functions of the p-irreducible representations, then θ_L^1 is taken as giving a new symmetry function for the $p+1$ irreducible representation, i.e.,

$$\chi_L^{p+1,11} = \theta_L^1. \tag{22}$$

If S_L^R is zero for some L index but non-zero for others, then for those L values with zero scalar products we write

$$\chi_L^{R,(\lambda_{\max}+1)1} = \theta_L^1. \tag{23}$$

The final inequality, (21c), indicates that θ_L^1 belongs to the Rth irreducible representation and a new χ can be found by writing

$$\theta_L^1 = \sum_{\lambda}^{(\lambda_{\max}+1)} a_\lambda \chi_L^{R,\lambda 1}. \tag{24}$$

That is, by the Gram–Schmidt orthogonalisation procedure we obtain $\chi_L^{R,(\lambda_{\max}+1)1}$.

The degenerate molecular orbitals have an additional complication associated with the arbitrary phase of the decomposed function θ_L^α

$$\theta_L^\alpha = \sum_{\lambda} \sum_{\beta}^{g} a_\lambda^{\alpha\beta} \chi_L^{Q,\lambda\beta}. \tag{25}$$

However, the interpretation of the scalar products is analogous to the non-degenerate case, namely,

$$\text{(i)} \qquad S_L^R = g, \tag{26a}$$

$$\text{(ii)} \qquad S_L^R = 0, \tag{26b}$$

$$\text{(iii)} \qquad 0 < S_L^R < g. \tag{26c}$$

These conditions are interpreted in the same manner as for the non-degenerate case. For example, for θ_L^α being orthogonal to the symmetry functions we put either

$$\chi_L^{p+1,1\alpha} = \theta_L^\alpha, \qquad \alpha = 1, \dots, g, \tag{27}$$

or

$$\chi_L^{R,(\lambda_{\max}+1)\alpha} = \theta_L^\alpha, \qquad \alpha = 1, \dots, g, \tag{28}$$

which ever is appropriate. Note (28) will cause phase problems but these are resolved by the second part of the program.

A slightly different orthogonalisation procedure is needed for (iii) so as to retain the correct phase of $\chi_L^{R,(\lambda_{\max}+1)}$, this procedure is outlined in Appendix I.

The program analyses each eigenvector in turn, including all the virtual and occupied orbitals, so as to ensure that a complete set of symmetry functions χ are found.

2.2b. *Refinement of the Symmetry Functions*

The blocked Fock matrix is given by

$$F^B = F_{L,L'}^{R,\Lambda;R',\Lambda'} = (\mathbf{T}_L^{R,\Lambda})^+ \mathbf{F}(\mathbf{T}_{L'}^{R',\Lambda'}), \tag{29}$$

where Λ is a combination of the λ and α superscripts, and from group theory $\mathbf{F}^B$ should be null when

(i) $R \neq R'$,

(ii) $\alpha \neq \alpha'$.

During the first eigenvalue determination using the symmetry-adapted functions to block-diagonalise the Fock matrix, the program checks that the off-diagonal $\mathbf{F}^B$ matrices between the irreducible representations of the same degeneracy are indeed zero. An appropriate threshold for finding non-zero $\mathbf{F}_B$ blocks was of the order 10^{-9} for various Ni_6 clusters, and we expect systems with larger basis sets to require slightly larger thresholds. If a non-zero off-diagonal $\mathbf{F}_B$ is found between R and R', the sets of χ^R and $\chi^{R'}$ are merged and treated henceforth as belonging to the same irreducible representation. For example, this situation occurs for diatomic nickel oxide. In NiO the d_π overlap with the other atomic orbitals with similar symmetry may be so small that the Hückel Hamiltonian generates a π eigenvector completely localised on the Ni d-orbital. This d–π eigenvector is orthogonal to all the other χ^π symmetry functions and the first part of the program causes the $\chi^{d\pi}$ function to be treated as belonging to a separate irreducible representation. The addition of more π

integrals into the Fock Hamiltonian enables a greater mixing between the d–π and other π-orbitals and now the two sets of functions can be grouped together.

In Section 2.2a we noted that there can be some difference of phases for the degenerate χ^d functions. There can also be phase problems when merging χ^R and $\chi^{R'}$ as required for the above. To illustrate the alignment, consider the doubly degenerate function $\chi_{L'}^{R;\Lambda'}$ which is out of phase with $\chi_L^{R,\Lambda}$. The transformed Fock matrix is given as

$$\begin{aligned} F_{L,L'}^{R,\Lambda;R,\Lambda'} &= (\mathbf{T}_L^{R,\Lambda})\,\mathsf{F}(\mathbf{T}_{L'}^{R;\Lambda'}) \\ &\neq 0 \qquad \text{when} \quad \alpha \neq \alpha', \alpha = 1, 2, \alpha' = 1, 2. \end{aligned} \tag{30}$$

The out-of-phase vector $\mathbf{T}_{L'}^{R;\Lambda'}$ can be written as a sum of in-phase vectors

$$\mathbf{T}_{L'}^{R;\lambda'1'} = \sin\gamma \mathbf{T}_{L'}^{R;\lambda'1} + \cos\gamma \mathbf{T}_{L'}^{R;\lambda'2} \tag{31a}$$

and

$$\mathbf{T}_{L'}^{R;\lambda'2'} = \cos\gamma \mathbf{T}_{L'}^{R;\lambda'1} - \sin\gamma_l \mathbf{T}_{L'}^{R;\lambda'2} \tag{31b}$$

which on substituting into (30) gives

$$\tan\gamma = \frac{F^{\lambda 1;\lambda'1'}}{F^{\lambda 1;\lambda'2'}} = -\frac{F^{\lambda 2;\lambda'2'}}{F^{\lambda 2;\lambda'1'}}, \tag{32}$$

where the indices R, L and L' have been dropped for convenience, enabling the set of in-phase vectors to be determined. The alignment of vectors with higher degeneracy is given in Appendix II.

A final test is required on the sign of the degenerate symmetry-adapted functions, that is a phase difference of 180° is not detected in the off-diagonal F_B. This is performed by checking the signs of

$$F_{L,L'}^{R,\lambda\alpha;R,\lambda'\alpha}; \qquad \alpha = 1,\dots, g, \tag{33}$$

for one complete row or column in each of the g diagonal F_B matrices.

3. DISCUSSION

In this section we demonstrate the computation savings made through using symmetry blocking. The algorithms described above have been implemented in a computer program.[1] Table I shows the relative computational times for some MINDO calculations on clusters of Ni atoms. In the usual semi-empirical calculation, where the Fock matrix is directly diagonalised, the time required for a MINDO calculation is essentially dependent on the basis set size and independent of

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[1] The authors plan to eventually submit the program to QCPE.

TABLE I

The Relative Computer Times for Some MINDO Calculations

				Relative computer times		
					Diagonalisation with symmetry blocking	
Molecule	Point group	Total number of basis functions	Number of functions in irreducible representation	Diagonalisation	A	B
Ni_6	C_s	54	$30A' + 24A''$	100	60	56
Ni_6	O_h	54	$3A_{1g} + 1A_{2g} + 1A_{2u}$ $+ 1E_g + 4E_u + 2T_{1g}$ $+ 3T_{2g} + 5T_{1u} + 3T_{2u}$	100	37	33
Ni_5	C_{4v}	45	$9A_1 + 3A_2 + 7B_1$ $+ 4B_2 + 11E$	100	44	39
Ni_2	$D_{\infty h}$	18	$3\Sigma_g^+ + 3\Sigma_u^- + 2\Pi_g$ $+ 2\Pi_u + 1\Delta_g + 1\Delta_u$	100	79	79

Note. (A) Calculation includes the time to determine the symmetry-adapted basis function. (B) The symmetry-adapted functions are read at the start of the calculation.

the atoms involved, except in that these atoms will determine the basis set size. Hence the following discussion will apply to any molecule or cluster.

The first point to note from Table I is that the additional time required for the initial determination of the symmetry-adapted functions is only a minor contribution to the total computational time. More specifucally, for the larger molecules Ni_5 and Ni_6 approximately 10 sec (on an IBM 370/155 machine) is required to obtain the symmetry-adapted functions, whereas for Ni_2 approximately 0.1 sec is required.

Secondly, Table I indicates that our procedure gives the better computational efficiency for molecules with higher symmetry. Such a result is not unexpected as the symmetry-adapted functions from groups with high symmetry span more different irreducible representations, giving rise to smaller blocked Fock matrices $\mathbf{F}_B$, than those obtained in the low symmetry case: for example, compare, in Table I, the number of symmetry-adapted functions in each irreducible representation for the two Ni_6 clusters. There is a surprising reduction in the computer time needed for the low symmetry case of Ni_6 with C_s symmetry. For this molecule, the original 54×54 Fock matrix is blocked into two matrices of size 30×30 (for the A' irreducible representation) and 24×24 (for A'') accounting for the computational gain.

Further improvements in our computational times could be obtained by a more efficient blocking transformation. At present the blocked Fock matrix $\mathbf{F}^B$ is obtained from the matrix multiplications required by Eq. (29). We hope to develop a better blocking procedure using the approach of Pitzer *et al.* using the theorem that symmetry related atomic orbital integrals make equal contribution to the symmetric orbital integrals [8].

Finally the value of making explicit symmetry considerations for Ni_2 might be questioned. However, as mentioned in the introduction, the advantage here is that we can have a greater control over the orbital occupancy; this is demonstrated elsewhere [3].

APPENDIX I: ORTHOGONALISATION OF DEGENERATE SYMMETRY FUNCTIONS

Extending Eq. (20) to the degenerate case, we have for the decomposed function θ

$$\theta_L^\alpha = \sum_\beta \left(\sum_\lambda^{\lambda_{\max}} a_\lambda \chi_L^{R,\lambda\beta} + a_{\lambda_{\max+1}} \chi_L^{R,\lambda_{\max+1}\beta} \right) b^{\beta\alpha}, \tag{AI.1}$$

where $\chi_L^{R,\lambda_{\max+1}\beta}$, the new symmetry-adapted function, is in-phase with the other functions of the Rth irreducible representation. $b^{\alpha\beta}$ is given by

$$b^{\alpha\beta} a_\lambda = (\chi_L^{R,\lambda\alpha}, \theta_L^\beta) \tag{AI.2}$$

and forms a $g \times g$ unitary matrix $\mathbf{B}$ which aligns the phases of θ and χ. Hence the required orthogonal symmetry function is obtained from

$$\chi_L^{R,\lambda_{\max+1}} = \frac{1}{a_{\lambda_{\max+1}}} \left(\mathbf{B}^{-1} \boldsymbol{\theta}_L - \sum_\lambda^{\lambda_{\max}} a_\lambda \chi_L^{R,\lambda} \right). \tag{AI.3}$$

APPENDIX II: ALIGNMENT OF PHASES FOR ORTHOGONAL DEGENERATE SYMMETRY FUNCTIONS

Let the out-of-phase degenerate functions for the Rth irreducible representation be labelled as $\chi_\mu'^\alpha$ and the in-phase functions as χ_μ^α, where for convenience we drop the labels R, λ, l and a. The two functions are related

$$\chi_\mu'^\alpha = \sum_\beta^g \chi_\mu^\beta b^{\beta\alpha} \tag{AII.1}$$

which in matrix notation is

$$\mathbf{T}'_\mu = \mathbf{T}_\mu \mathbf{B}, \tag{AII.2}$$

where $\mathbf{T}_\mu = (\mathbf{T}_\mu^1 \mathbf{T}_\mu^2 \cdots \mathbf{T}_\mu^g)$, and $\mathbf{B}$ is a $g \times g$ unitary matrix similar to that of Appendix I.

An out-of-phase transformed Fock matrix $\mathbf{F}'^B$ is obtained from

$$(\mathbf{F}'^B)_{\mu\lambda}^{\alpha\beta} = (\mathbf{T}_\mu'^\alpha)^+ \, \mathbf{F} \mathbf{T}_\lambda^\beta, \tag{AII.3}$$

where χ_{λ}^{β} is a different symmetry function, with the correct phase, belonging to the Rth irreducible representation. Substituting (AII.2) into (AII.3) and rearranging gives

$$\mathbf{B} = \mathbf{F}'^{B}(\mathbf{F}^{B})^{-1}, \qquad \text{(AII.4)}$$

where $\mathbf{F}^{B}$ is a correctly blocked Fock matrix, in fact a unit matrix multiplied by a constant. Hence the inverse of $\mathbf{B}$ can be found and χ_{μ}^{α} determined.

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