

Factorization of the Hückel Hamiltonian Matrix for Highly Symmetrical Molecules

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A simple approach to the group-theoretical factorizing of the Hamiltonian matrix of highly symmetrical molecules is presented. This approach, which is based on the Lanczos method, requires only a symmetry-adapted linear combination (SALC) for each category of irreducible representation (IR) of the molecular point-group, while it reduces the size of the problem by more than one order of magnitude. We demonstrate the treatment by applying it to the study of electronic structures of the Goldberg type-II fullerenes, C_{80} , C_{180} , C_{320} , C_{500} and C_{980} within the Hückel tight-binding framework. The results, in terms of the factor characteristic polynomial (or the subspectrum) for each category of irreducible representation, are presented for these giant molecules.

INTRODUCTION

Stimulated by the experimental observation of Buckminsterfullerene¹ and the spheroidal concentric graphitic structures,^{2,3} the energetics and configurations of I_h -symmetrical carbon cages (Goldberg type-I and type-II fullerenes)^{4–7} have been the focus of numerous theoretical investigations.^{5–40} Among them, calculations^{8–29} based on the Hückel (tight-binding) molecular orbital theory provide preliminary results for the topological analysis of their stability.

The central theme of quantum mechanical calculations for a molecule is known to be the determination of the eigenvalues and eigenvectors of its

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Hamiltonian. With the Hückel approximation, the Hamiltonian matrix is of dimension N , the number of atoms. Consequently, when we are dealing with giant molecules, for instances, C_{720} and C_{980} direct diagonalization of the Hückel Hamiltonian matrix becomes unfavorable due to the limited capacity of an ordinary computer. One of the traditional ways of reducing this difficulty is to factorize (reduce) the Hamiltonian matrix into the block-diagonal form and to solve the eigenproblem of smaller blocks.

Thus, the problem arises of how to factorize the Hamiltonian matrix in an efficient way. There have been several solutions to this problem thus far.¹⁹⁻²⁹ In this work, we prefer a treatment based on the Lanczos method. Its efficiency and facility will be illustrated by several giant Goldberg fullerenes.

APPROACH

First, let us give a brief review of the group factorization problem of the Hamiltonian matrix within the Hückel framework. Assume ϕ_i ($i = 0, 1, \dots, N-1$) are the basis functions for the molecule under consideration. The Hamiltonian matrix will be of dimension N and the matrix elements are

$$H_{ij} = \langle \phi_i | \hat{H} | \phi_j \rangle . \quad (1)$$

The basis functions $\{\phi_i\}$ span a reducible representation space of the Hamiltonian, which decomposes to a sum of irreducible representations

$$\Gamma = \oplus \sum_{\alpha=1}^h f_{\alpha} \Gamma_{\alpha} \quad (2)$$

where Γ_{α} stands for the α -th irreducible representation (IR) of the point group and f_{α} denotes its repetitive frequency, and the sum runs over the h categories of IRs of the point group. The structure of Γ implies that, on adopting a set of mutually-orthogonal symmetry-adapted linear combinations of atomic orbitals (SALCs) as new basis functions, the Hamiltonian matrix H decomposes into the direct sum of submatrices

$$H = \oplus \sum_{\alpha=1}^h l_{\alpha} H_{\alpha} \quad (3)$$

where l_{α} is the dimensionality of the irreducible representation Γ_{α} and H_{α} the corresponding Hamiltonian submatrix of order f_{α} . At the same time, the secular determinant of the molecule, $\det(xI-H)$, is factorized in the following manner

$$\det(xI-H) = \prod_{\alpha=1}^h [\det(xI_{\alpha} - H_{\alpha})]^{l_{\alpha}} = \prod_{\alpha=1}^h [P_{\alpha}(x)]^{l_{\alpha}}. \quad (4)$$

It is obvious that the f_{α} roots of the α -th sub-determinant equation

$$P_{\alpha}(x) = \det(xI_{\alpha} - H_{\alpha}) = 0 \quad (5)$$

will make up the subspectrum for IR Γ_{α} and each of the roots will be l_{α} -degenerate in the entire molecular energy spectrum.

Now, it is clear that the essential step to attain the factorization described by Eq. (3) or (4) is to find a complete set of SALCs to be employed as new basis functions. As far as we know, constructing all the SALCs required for the factorization has been a somewhat cumbersome task in the case of highly symmetrical giant molecules, either through the linear combinations of the spherical harmonics⁴¹⁻⁴³ or by utilizing the complete projection operator technique.⁴⁴ However, as it will be seen in this paper, if one applies the Lanczos method,^{45,46} all the SALCs required can be easily generated in a recursive way. As a result, the Hamiltonian matrix will be readily factorized.

As we know, the Lanczos method can be applied to the tridiagonalization of the Hamiltonian matrix. It begins with an arbitrary starting state u_0 , rendering a set of mutually orthogonal states $\{u_i\}$ through the following recursive process. The first of the states u_i is derived as follows,

$$u_1 = H u_0 - a_0 u_0 \quad (6)$$

where coefficient a_0 can be determined in accordance with the orthogonality condition, *i.e.* $\langle u_i | u_j \rangle = 0$, for $i \neq j$. So we have

$$a_0 = \frac{\langle u_0 | H | u_0 \rangle}{\langle u_0 | u_0 \rangle}. \quad (7)$$

The second and the subsequent states are constructed one by one by the recursion formula

$$u_{k+1} = H u_k - a_k u_k - b_k u_{k-1} \quad (8)$$

where coefficients a_k , b_k are determined by

$$a_k = \frac{\langle u_k | H | u_k \rangle}{\langle u_k | u_k \rangle}, \quad b_k = \frac{\langle u_{k-1} | H | u_k \rangle}{\langle u_{k-1} | u_{k-1} \rangle}. \quad (9)$$

The recursion process will terminate at some step when $u_n = 0$. In this way, one obtains a set of states $\{u_i\}$. In quantum mechanics, one prefers the normalized states defined as

$$\{|k\rangle\} = \frac{u_k}{\langle u_k|u_k\rangle^{1/2}}. \quad (10)$$

In terms of this new orthogonal set $\{|k\rangle\}$, the Hamiltonian matrix corresponds to a tridiagonal form, where only the diagonals and their nearest neighboring entries are not equal to zero, *i.e.*,

$$H_{mm} = \langle m|H|m\rangle = \frac{\langle u_m|H|u_m\rangle}{\langle u_m|u_m\rangle} = \alpha_m \quad (11)$$

$$H_{m-1,m} = H_{m,m-1} = \langle m-1|H|m\rangle = \frac{\langle u_{m-1}|H|u_m\rangle}{\langle u_{m-1}|u_{m-1}\rangle^{1/2} \langle u_m|u_m\rangle^{1/2}} = b_m^{1/2} \quad (12)$$

$$H_{mm'} = 0, \quad \text{if } |m - m'| > 1. \quad (13)$$

Moreover, it can be easily proved that the above transformation process preserves the symmetry of the starting state, *i.e.* if u_0 is a SALC of irreducible representation Γ_α , the derived states u_1, u_2, \dots, u_n are also SALC belonging to the same row of irreducible representation Γ_α . In this way, *the Lanczos method can be generally applied to deriving f_α SALCs belonging to the same row of irreducible representation, Γ_α .*

Now, this approach for the group-theoretical factorizing of the Hamiltonian can be better summarized as a three-step scheme:

- (1) Construct a SALC for each category of irreducible representation;
- (2) For each category of irreducible representation Γ_α , use the corresponding SALC as the starting state to start the recursive process, and derive the other SALC belonging to the same row of irreducible representation, evaluate the corresponding tridiagonal Hamiltonian submatrix H_α of dimension f_α . As a whole, the Hamiltonian matrix of the molecule falls into the block-diagonal form as in Eq. (3).

- (3) Solve the eigenproblem of each tridiagonal submatrix separately.

At this stage, the factor characteristic polynomials and, thus, the sub-spectrum referring to each category of IR are obtained.

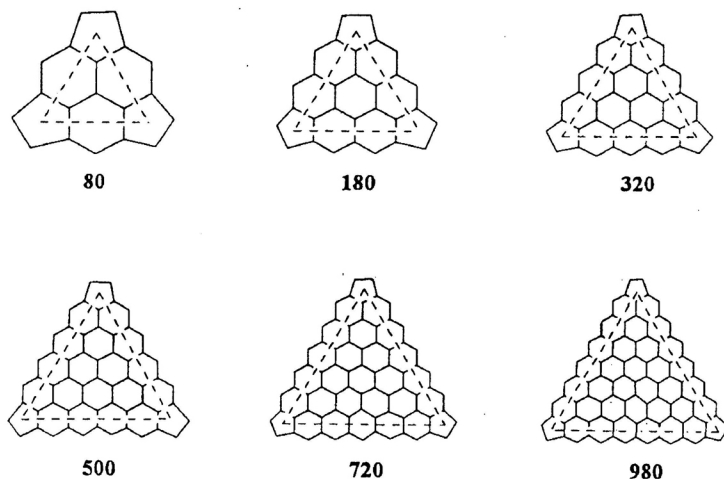


Figure 1. Structural units of Goldberg type-II fullerenes.

TREATMENT OF GOLDBERG TYPE-II FULLERENES

In the 30's, Goldberg⁴ noted a class of polyhedra possessing only trivalent vertices, and only pentagonal and hexagonal faces. He showed that there are exactly twelve pentagons and that the remaining faces are hexagonal. The number of vertices of these polyhedrons, N , is given by $20(a^2 + ab + b^2)$, with a, b non-negative integers.^{9,13} If a equals b (type-I, $N = 60k^2$) or ab equals 0 (type-II, $N = 20k^2$), the polyhedron will be of I_h symmetry. If carbon atoms are placed on the vertices of these polyhedrons, Goldberg fullerenes result. In a topological sense, the carbon atoms of Goldberg fullerenes are distributed on the twenty triangles of a master icosahedron. In Figure 1, one of the triangles is depicted for six Goldberg type-II fullerenes, C_{20k^2} ($k = 2, 3, \dots, 7$).

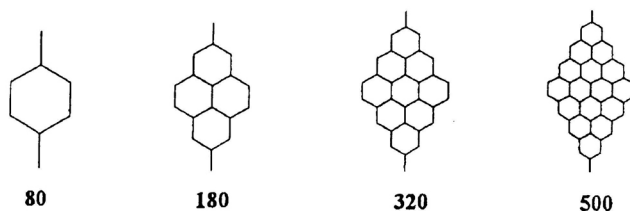


Figure 2. Repeat units of Goldberg type-II fullerenes (each repeat unit is made up of two neighboring structural units).

Resulting from the S_{10} subgroup symmetry of these molecules, a fragment with $2k^2$ carbon atoms (see Figure 2) can be regarded as the repeat unit for C_{20k^2} , and the carbon atoms can be labelled in a circulant way so that the Hückel Hamiltonian matrix is a circulant matrix⁴⁷⁻⁴⁹ as follows:

$$H = \begin{pmatrix} U & V & W & 0 & 0 & 0 & 0 & 0 & W^T & V^T \\ V^T & U & V & W & 0 & 0 & 0 & 0 & 0 & W^T \\ W^T & V^T & U & V & W & 0 & 0 & 0 & 0 & 0 \\ 0 & W^T & V^T & U & V & W & 0 & 0 & 0 & 0 \\ 0 & 0 & W^T & V^T & U & V & W & 0 & 0 & 0 \\ 0 & 0 & 0 & W^T & V^T & U & V & W & 0 & 0 \\ 0 & 0 & 0 & 0 & W^T & V^T & U & V & W & 0 \\ 0 & 0 & 0 & 0 & 0 & W^T & V^T & U & V & W \\ W & 0 & 0 & 0 & 0 & 0 & W^T & V^T & U & V \\ V & W & 0 & 0 & 0 & 0 & 0 & W^T & V^T & U \end{pmatrix} \quad (14)$$

where U, V, W, V^T, W^T are all of dimension $2k^2$, U describes the internal connectivity in the repeat unit in Figure 2, V and W describe the connectivity between the neighboring repeat units, and V^T, W^T are their transposes.

It can be easily proved that this representative of the Hamiltonian is a reducible one with respect to I_h group, decomposing according to the following formula

$$\begin{aligned} \Gamma_k = & \frac{k^2 + 3k + 2\delta_{k, 3m\pm 1}}{6} A_g \oplus \frac{k^2 - k}{2} T_{1g} \oplus \frac{k^2 - k}{2} T_{2g} \oplus \frac{2k^2 + \delta_{k, 3m\pm 1}}{3} G_g \\ & \oplus \frac{5k^2 + 3k - 2\delta_{k, 3m\pm 1}}{6} H_g \oplus \frac{k^2 - 3k + 2\delta_{k, 3m\pm 1}}{6} A_u \oplus \frac{k^2 + k}{2} T_{1u} \\ & \oplus \frac{k^2 + k}{2} T_{2u} \oplus \frac{2k^2 + \delta_{k, 3m\pm 1}}{3} G_u \oplus \frac{5k^2 - 3k - 2\delta_{k, 3m\pm 1}}{6} H_u \end{aligned} \quad (15)$$

The repetitive frequencies of IRs in Eq. (15), which depend on k , are collected up to $k \leq 7$ in Table I. One may notice that the A_u irreducible representation doesn't appear in C_{80} and C_{180} , but does appear one or more times in C_{320} and larger cages.

Now, we apply the approach, described in the last section, to the factorization of the Hamiltonian matrix for these fullerene molecules. In a previous work²⁸ by using the projection operator technique, we constructed a set of SALCs as starting states for the nine IRs occurring in C_{80} which are contributed by the sixty equivalent atomic orbitals on 12 pentagons. These

TABLE I

Repetitive frequencies of irreducible representations for Goldberg type-II fullerenes within the Hückel tight-binding approximation

<i>k</i>	<i>N</i> (=20 <i>k</i> ²)	<i>A_g</i>	<i>T_{1g}</i>	<i>T_{2g}</i>	<i>G_g</i>	<i>H_g</i>	<i>A_u</i>	<i>T_{1u}</i>	<i>T_{2u}</i>	<i>G_u</i>	<i>H_u</i>
2	80	2	1	1	3	4	0	3	3	3	2
3	180	3	3	3	6	9	0	6	6	6	6
4	320	5	6	6	11	15	1	10	10	11	11
5	500	7	10	10	17	23	2	15	15	17	18
6	720	9	15	15	24	33	3	21	21	24	27
7	980	12	21	21	33	44	5	28	28	33	37

starting states can be also applied to higher members of C_{20k²} due to the structural similarity, that is, the sixty atoms on the 12 pentagons of these cages are also equivalent and distributed analogously on an icosahedron (see Figure 1.). As a result, similar SALCs can be constructed as the starting states for any higher member of C_{20k²}, which are also linear combinations of atomic orbitals on pentagons, with the same coefficients of SALCs of C₈₀, which were tabulated in ref. 28. The starting state for A_u which appears in C₃₂₀ and larger ones can also be constructed with the 120 atoms which are

TABLE II

Factor characteristic polynomials (FCPs) of C₈₀ and their related eigenvalues

IR	FCPs	Eigenvalues
<i>A_g</i>	$x^2 - 2x - 3$	3, -1
<i>T_{1g}</i>	$x + \frac{1 - \sqrt{5}}{2}$	0.618
<i>T_{2g}</i>	$x + \frac{1 + \sqrt{5}}{2}$	-1.618
<i>G_g</i>	$x^3 + x^2 - 4x + 1$	1.377, 0.274, -2.651
<i>H_g</i>	$x^4 - x^3 - 6x^2 + 3x + 7$	2.473, 1.463, -1, -1.935
<i>T_{1u}</i>	$x^3 - \frac{3 + \sqrt{5}}{2}x^2 - (4 - \sqrt{5})x + \frac{9 - \sqrt{5}}{2}$	2.818, 1, -1.200
<i>T_{2u}</i>	$x^3 - \frac{3 - \sqrt{5}}{2}x^2 - (4 + \sqrt{5})x + \frac{9 + \sqrt{5}}{2}$	2.081, 1, -2.699
<i>G_u</i>	$x^3 + x^2 - 4x - 3$	1.912, -0.714, -2.199
<i>H_u</i>	$x^2 + x - 1$	0.618, -1.618

TABLE III

Factor characteristic polynomials (FCPs) of C_{180} and their related eigenvalues

IR	FCPs	Eigenvalues
A_g	$x^3 - 3x^2 - 3x + 9$	3, 1.732, -1.732
T_{1g}	$x^3 + \frac{3 - \sqrt{5}}{2}x^2 - \frac{3 + \sqrt{5}}{2}x - \frac{3 - \sqrt{5}}{2}$	1.514, -0.144, -1.752
T_{2g}	$x^3 + \frac{3 + \sqrt{5}}{2}x^2 - \frac{3 - \sqrt{5}}{2}x - \frac{3 + \sqrt{5}}{2}$	0.916, -1.251, -2.283
G_g	$x^6 + x^5 - 9x^4 - 5x^3 + 20x^2 + 6x - 11$	2.202, 1.475, 0.737, -1.078, -1.508, -2.828
H_g	$x^9 - 2x^8 - 12x^7 + 22x^6 + 44x^5 - 72x^4 - 53x^3 + 75x^2 + 18x - 21$	2.762, 2.270, 1.551, 1, 0.595, -0.698, -1.099, -1.913, -2.470
T_{1u}	$x^6 - \frac{3 + \sqrt{5}}{2}x^5 - (9 - \sqrt{5})x^4 + \frac{21 + 5\sqrt{5}}{2}x^3 + \frac{41 - 9\sqrt{5}}{2}x^2 - (14 + 3\sqrt{5})x - \frac{23 - 9\sqrt{5}}{2}$	2.919, 1.980, 1.269 -0.067, -1.386, -2.098
T_{2u}	$x^6 - \frac{3 - \sqrt{5}}{2}x^5 - (9 + \sqrt{5})x^4 + \frac{21 - 5\sqrt{5}}{2}x^3 + \frac{41 + 9\sqrt{5}}{2}x^2 - (14 - 3\sqrt{5})x - \frac{23 + 9\sqrt{5}}{2}$	2.569, 1.889, 1.157, -0.920, -1.464, -2.849
G_u	$x^6 + x^5 - 9x^4 - 7x^3 + 18x^2 + 6x - 9$	2.503, 1.123, 0.724, -0.940, -1.799, -2.613
H_u	$x^6 + x^5 - 6x^4 - 4x^3 + 9x^2 + 3x - 3$	1.864, 1.162, 0.512, -0.817, -1.465, -2.257

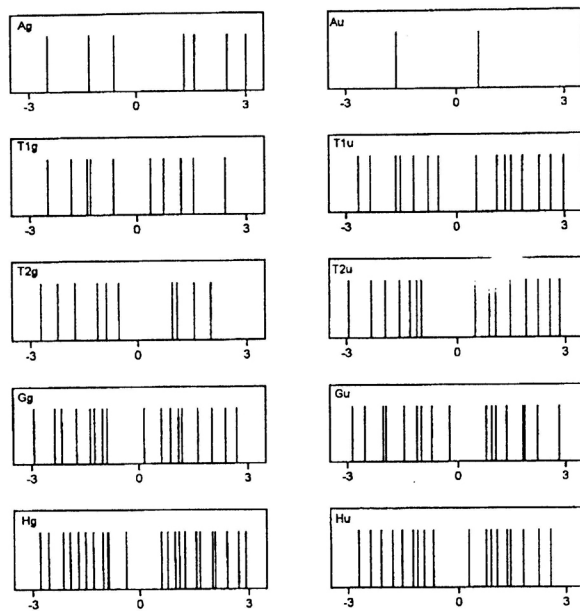
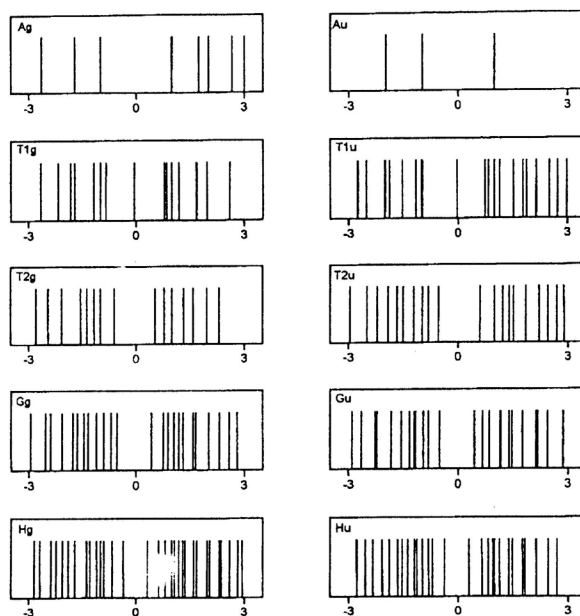
the second nearest neighbors with respect to the pentagons by the projection operator technique.

Due to the circulant property of the Hamiltonian matrix (see Eq. (14)), only smaller matrices U , V , W and their transposes will be used in the factorization. On the other hand, as indicated in Table I, the dimension of the resulting Hamiltonian submatrices will be no larger than k^2 (one twentieth of the dimension of the Hamiltonian matrix). Therefore, this approach reduces the size of the problem by more than one order of magnitude. In reality, it takes only several minutes to attain the factorization for giant molecules such as C_{720} and C_{980} on a PC 486/33. In Tables II-IV, the factor characteristic polynomials (FCPs) in analytical form and their related eigenvalues are presented for C_{80} , C_{180} and C_{320} ; while for the other three Goldberg type-II fullerenes, the subspectra instead of FCPs are given to save space.

TABLE IV

Factor characteristic polynomials (FCPs) of C_{320} and their related eigenvalues

IR FCPs	Eigenvalues
A_g $x^5 - 3x^4 - 6x^3 + 18x^2 + 5x - 15$	3, 2.236, 1, -1, -2.236
T_{1g} $x^6 + \frac{3 - \sqrt{5}}{2}x^5 - \frac{11 + \sqrt{5}}{2}x^4 - (6 - 2\sqrt{5})x^3 + \frac{17 + \sqrt{5}}{2}x^2 + (5 - 2\sqrt{5})x - \frac{9 - \sqrt{5}}{2}$	2.122, 1, 0.765, -0.708, -1.305, -2.256
T_{2g} $x^6 + \frac{3 + \sqrt{5}}{2}x^5 - \frac{11 - \sqrt{5}}{2}x^4 - (6 + 2\sqrt{5})x^3 + \frac{17 - \sqrt{5}}{2}x^2 + (5 + 2\sqrt{5})x - \frac{9 + \sqrt{5}}{2}$	1.559, 1, 0.575, -1.285, -1.898, -2.570
G_g $x^{11} + x^{10} - 16x^9 - 13x^8 + 89x^7 + 59x^6 - 211x^5 - 111x^4 + 207x^3 + 84x^2 - 65x - 20$	2.538, 2.083, 1.555, 1.122, 0.740, -0.281, -0.806, -1.226, -1.772, -2.054, -2.898
H_g $x^{15} + 2x^{14} - 22x^{13} + 41x^{12} + 190x^{11} - 323x^{10} - 834x^9 + 1255x^8 + 2020x^7 - 2579x^6 - 2716x^5 + 2767x^4 + 1887x^3 - 1398x^2 - 526x + 239$	2.866, 2.579, 2.120, 1.669, 1.541, 1.150, 1, 0.331, -0.784, -1, -1.216, -1.491, -1.736, -2.341, -2.689
A_u $x + 1$	-1
T_{1u} $x^{10} - \frac{5 + \sqrt{5}}{2}x^9 - \frac{27 - 3\sqrt{5}}{2}x^8 + (33 + 5\sqrt{5})x^7 + \frac{117 - 33\sqrt{5}}{2}x^6 - \frac{275 + 29\sqrt{5}}{2}x^5 - (99 - 59\sqrt{5})x^4 + (208 + 105\sqrt{5})x^3 + \frac{147 - 153\sqrt{5}}{2}x^2 - 101x - \frac{41 - 65\sqrt{5}}{2}$	2.955, 2.402, 1.937, 1.264, 1, 0.578, -1, -1.054, -1.992, -2.473
T_{2u} $x^{10} - \frac{5 - \sqrt{5}}{2}x^9 - \frac{27 + 3\sqrt{5}}{2}x^8 + (33 - 5\sqrt{5})x^7 + \frac{117 + 33\sqrt{5}}{2}x^6 - \frac{275 - 29\sqrt{5}}{2}x^5 - (99 + 59\sqrt{5})x^4 + (208 - 105\sqrt{5})x^3 + \frac{147 + 153\sqrt{5}}{2}x^2 - 101x - \frac{41 + 65\sqrt{5}}{2}$	2.754, 2.341, 1.860, 1.438, 1, -0.632, -1, -1.471, -1.998, -2.910
G_u $x^{11} + x^{10} - 16x^9 - 13x^8 + 89x^7 + 51x^6 - 219x^5 - 71x^4 + 239x^3 + 20x^2 - 89x + 12$	2.717, 1.817, 1.342, 1.279, 0.710, 0.148, -0.925, -1.458, -1.587, -2.271, -2.774
H_u $x^{11} + 2x^{10} - 12x^9 - 23x^8 + 49x^7 + 89x^6 - 84x^5 - 140x^4 + 63x^3 + 88x^2 - 18x - 17$	2.335, 1.844, 1.254, 0.883, 0.689, -0.466, -1, -1.286, -1.646, -2.056, -2.552

Figure 3. Hückel subspectra of C_{500} .Figure 4. Hückel subspectra of C_{720} .

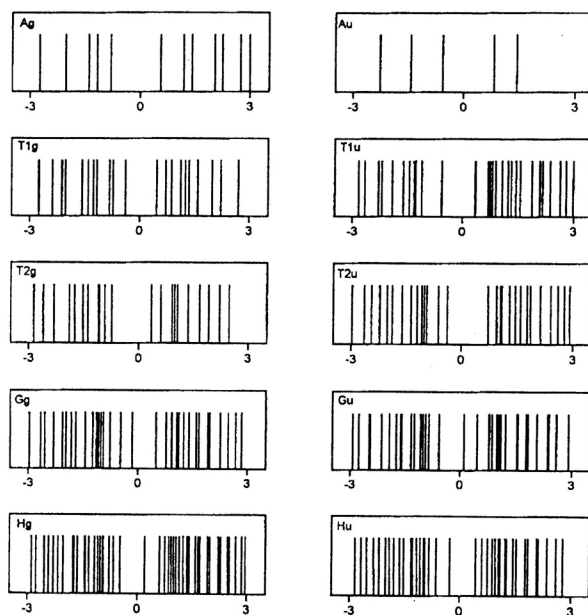


Figure 5. Hückel subspectra of C_{980} .

DISCUSSION AND CONCLUSION

From the calculations in the last section, it is quite clear that upon utilizing the Lanczos method, a series of Symmetry-adapted Linear Combinations (SALCs) can be generated recursively from one SALC, and thus the Hückel Hamiltonian matrix of a highly symmetrical molecule can easily be group factorized into a direct sum of the smallest submatrices. Therefore, in this paper, we have suggested a simple but efficient approach for solving the Hückel eigenvalue problem for highly symmetrical molecules.

To our knowledge, besides this approach, there have already been several other approaches dealing with the Hückel eigenvalue problem of fullerenes: the direct diagonalization of the Hamiltonian matrix; reducing the molecule into subsystems by the use of its Z_2 or S_{10} symmetry;¹⁷⁻²² deriving the characteristic polynomial referring to each irreducible representation on the basis of the character table and the multiplication table,²³ and so on. We notice that the approach advanced by Lin and Nori^{25,26} also employs the Lanczos method. The chief difference between our work and theirs lies in the choice of the starting state. Our choice emphasizes the symmetry of the starting state in order to attain idealized factorization rendering maximum analytical results. It seems to us that the approach in this work may have a wider application and can be applied to other quantum chemical problems.

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REFERENCES

1. H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, and R. E. Smalley, *Nature* **318** (1985) 162.
2. S. Iijima, *J. Cryst. Growth* **50** (1980) 675.
3. D. Ugarte, *Nature* **359** (1992) 707.
4. M. Goldberg, *Tohoku Math. J.* **43** (1937) 104.
5. M. Yoshida and E. Osawa, *Fullerene Sci. Tech.* **1** (1993) 55.
6. D. York, J. P. Lu, and W. Yang, *Phys. Rev.* **B 49** (1994) 8526.
7. J. P. Lu and W. Yang, *Phys. Rev.* **B 49** (1994) 11421.
8. A. D. J. Haymet, *Chem. Phys. Lett.* **122** (1985) 421.
9. D. J. Klein, W. A. Seitz, and T. G. Schmalz, *Nature* **323** (1986) 703.
10. R. C. Haddon, L. E. Brus, and K. Raghavachari, *Chem. Phys. Lett.* **125** (1986) 459.
11. R. C. Haddon, L. E. Brus, and K. Raghavachari, *Chem. Phys. Lett.* **131** (1986) 165.
12. P. W. Fowler and J. Woolrich, *Chem. Phys. Lett.* **127** (1986) 78.
13. P. W. Fowler, *Chem. Phys. Lett.* **131** (1986) 444.
14. M. Ozaki and A. Takahashi, *Chem. Phys. Lett.* **127** (1986) 242.
15. M. D. Newton and R. E. Stanton, *J. Amer. Chem. Soc.* **108** (1986) 2469.
16. R. A. Davidson, *Theor. Chim. Acta* **58** (1981) 193.
17. J. R. Dias, *J. Chem. Educ.* **66** (1989) 1012.
18. E. Manousakis, *Phys. Rev.* **B 44** (1991) 10991.
19. Y. Deng and C. N. Yang, *Phys. Lett.* **A 170** (1992) 116.
20. T. T. Chou and C. N. Yang, *Phys. Lett.* **A 183** (1993) 221.
21. J. Liu, Y. H. Shao, and Y. S. Jiang, *Chem. Phys. Lett.* **210** (1993) 149.
22. H. Hosoya and Y. Tsukano, *Fullerene Sci. & Tech.* **2** (1994) 381.
23. W. B. Brown, *Chem. Phys. Lett.* **136** (1987) 128.
25. R. Friedberg, T. D. Lee, and H. C. Ren, *Phys. Rev.* **B 46** (1992) 14150.
25. Y.-L. Lin and F. Nori, *Phys. Lett.* **A 183** (1993) 214.
26. Y.-L. Lin and F. Nori, *Phys. Lett.* **B 49** (1994) 5020.
27. K. Balasubramanian and X. Liu, *J. Comput. Chem.* **9** (1988) 406.
28. C. G. Liu, Y. H. Shao, and Y. S. Jiang, *Chem. Phys. Lett.* **228** (1994) 131.
29. C. G. Liu, M. M. Wang, Y. H. Shao, and Y. S. Jiang, *Phys. Lett.* **A 196** (1994) 120.
30. T. G. Schmalz, W. A. Seitz, D. J. Klain, and G. E. Hite, *J. Amer. Chem. Soc.* **110** (1988) 1113.
31. H. W. Kroto and K. G. Mckay, *Nature* **331** (1988) 328.
32. K. G. Mckay, H. W. Kroto, and D. J. Wales, *J. Chem. Soc. Faraday Trans.* **88** (1992) 2815.
33. R. F. Curl and R. E. Smalley, *Scientific American* **265** (1991) 32.
34. M. Fujita, R. Saito, G. Dresselhaus, and M. S. Dresselhaus, *Phys. Rev.* **B 45** (1992) 13834.
35. A. C. Tang, Q. S. Li, C. W. Liu, and J. Li, *Chem. Phys. Lett.* **201** (1993) 465.
36. B. I. Dunlap, D. W. Brenner, J. W. Mintmire, R. C. Mowrey, and C. T. White, *J. Phys. Chem.* **95** (1991) 8737.
37. G. B. Adams, O. F. Sankey, J. B. Page, M. O'Keeffe, and D. A. Drabold, *Science* **256** (1992) 1792.
38. J. Tersoff, *Phys. Rev.* **B 46** (1992) 15546.
39. A. Maiti, C. J. Brabec, and J. Bernholc, *Phys. Rev. Lett.* **70** (1993) 3023.
40. D. A. Drabold and O. F. Sankey, *Phys. Rev. Lett.* **70** (1993) 3631.
41. A. J. Stone, *Mol. Phys.* **41** (1980) 1339.

42. A. J. Stone, *Inorg. Chem.* **20** (1981) 563.
43. A. J. Stone, *Polyhedron* **3** (1984) 1299.
44. F. A. Cotton, *Chemical Applications of Group Theory, 3rd Edition*, John Wiley & Sons, New York, 1990.
45. C. Lanczos, *J. Res. Natl. Bur. Stand.* **45** (1950) 255.
46. R. Haydock, in *Solid State Physics*, H. Ehrenreich, F. Seitz, and D. Turnbull, (Eds.), Academic Press, New York, 1980, Vol. 35
47. G. G. Hall, *Matrices and Tensors*, Pergamon Press, Oxford, 1963.
48. N. Trinajstić, *Chemical Graph Theory*, Vol. I. CRC Press, Boca Raton, 1983.
49. A. C. Tang, Y. S. Kiang, G. S. Yan, and S. S. Tai, *Graph Theoretical Molecular Orbitals*, Science Press, Beijing, 1986.

SAŽETAK

Faktorizacija matrice Hückelova hamiltoniana za visoko simetrične molekule

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Prikazan je jednostavan pristup faktorizaciji matrice hamiltoniana visoko simetričnih molekula s pomoću teorije grupa. Postupak, zasnovan na Lanczosovoj metodi, zahtijeva samo simetrijski prilagođenu linearnu kombinaciju (SALC) za svaku kategoriju ireducibilne reprezentacije (IR) molekulske grupe, a smanjuje veličinu problema za više od jednog reda veličine. Primjena tog postupka prikazana je u proučavanju elektronske strukture Goldbergovih fullerena II. tipa: C₈₀, C₁₈₀, C₃₂₀, C₅₀₀, C₇₂₀ i C₉₈₀, unutar Hückelove koncepcije jake veze. Rezultati za ove velike molekule prikazani su kao faktori karaktertističnog polinoma (odnosno podspektri) za svaku kategoriju ireducibilne reprezentacije.