Chapter 3

A method for construction of characteristic polynomials of linear graphs with arbitrary vertex- and edge-weights

3.1. Introduction

There exist quite a large number of methods for construction of characteristic polynomials (CP) of graphs . They may be classified into two major types, viz. (i) methods[96-102] that depend on counting of elementary subgraphs such as K_2' s and rings and (ii) methods[103-105] based on Cayley-Hamilton theorem and Newton's identities[106] which require calculation of traces of the various powers of the adjacency matrix (**A**) of the graph . While methods of type (i) bring out the combinatorial dependence of the CP coefficients on the graph structure, they are computationally difficult, particularly for large graphs with many fused rings . On the other hand methods of the type (ii) take into account such dependence only indirectly (traces of $\mathbf{A}^n$ may be correlated to self-returning walks[107] of length n), but are computationally facile . Randić[105] has shown how a method of the second type developed by Barakat[104] can be executed combinatorially through the use of selected Young diagrams after computing the traces of various powers of **A** . The object of the present chapter is to develop a computationally facile recursive method for evaluation of CP coefficients of undirected graphs having arbitrary vertex- and edge- weights after linearizing the graph through symmetry factorization where possible or through a graph linearization algorithm recently developed[108] which uses walks of unit length .

3.2. Method

The algorithm for linearizing a graph using walks of unit length may be found in ref.108 . Sometimes this is not required and the graph may be converted into an isospectral linear chain with proper edge- and vertex- weights by symmetry factorization . The present algorithm for building up the CP coefficients of a weighted linear chain is based on the recurrence relation

$$C_r^{(i)} = C_r^{(i-1)} + h_i\, C_{r-1}^{(i-1)} - k^2_{i-1,i}\, C_{r-2}^{(i-2)} \qquad \ldots (3.1)$$

$$C_0^{(i)} = 1\ ,$$

where $C_r^{(i)}$ means the r-th coefficient of the CP, $P(L_i\,;\,x)$, of a linear chain with i vertices :

$$P(L_i\,;\,x) = \sum_{r=0}^{i} (-1)^r\, C_r^{(i)}\, x^{i-r} \qquad \ldots (3.2)$$

where h_i is the weight of the i-th vertex and $k_{i-1,i}$ is the weight of the edge connecting the vertices labeled $i-1$ and i. Equation (3.1) can be derived from the Heilbronner recurrence relation[109] applied to a weighted linear chain from one end :

$$P(L_i ; x) = (x - h_i)\ P(L_{i-1} ; x) - k^2_{i-1,i}\ P(L_{i-2} ; x) \quad \ldots (3.3)$$

An easy procedure for executing the recursive work required by equation (3.1) follows :

1. Write down the coefficients (without sign) of the $(i - 1)$th chain in a row.
2. Multiply each coefficient by h_i and write them below the above row displacing one place to the right .
3. Multiply the coefficients of the $(i - 2)$th row by $-k^2_{i-1,i}$ and write them displaced two places to the right .
4. Add columnwise to get the coefficients $C_r^{(i)}$. Insert the sign of $(-1)^{r-1}$ before each $C_r^{(i)}$.

3.3. Illustrations

Case I : *Graphs Linearized by Symmetry Factorization*

(a) The graph $G_{3.1}$ (Fig.3.1) can be converted into mirror plane fragments $G_{3.1}^+$ and $G_{3.1}^-$ by McClelland's method[87-89] as shown in Fig.3.1 . This graph has been chosen because it contains as a subgraph the carbon atom skeleton of biphenylene, which was used by Hosoya[99] to illustrate his method of construction of CP coefficients . The building up of the CP coefficients of $G_{3.1}^+$ by the present method is shown in Table 3.1 . These yield, according to eqn.(3.2),

$$P (G_{3.1}^+ ; x) = x^8 - 5x^7 + 3x^6 + 17x^5 - 19x^4 - 17x^3 + 21x^2 + 5x - 5 \quad \ldots (3.4)$$

The CP of $G_{3.1}^-$ can be similarly constructed . It is noteworthy here that the portions of $G_{3.1}^+$ and $G_{3.1}^-$ up to the sixth vertex are the mirror plane fragments of $G_{3.2}$ (Fig. 3.1) and so

$$\begin{aligned} P(G_{3.2} ; x) &= P (L_6^+ ; x)\ P(L_6^- ; x) \\ &= (x^6 - 4x^5 + x^4 + 10x^3 - 6x^2 - 6x + 3) \times \\ &\quad (x^6 + 4x^5 - x^4 - 10x^3 - 6x^2 + 6x + 3) \\ &= x^{12} - 14x^{10} + 69x^8 - 154x^6 + 162x^4 - 72x^2 + 9 \quad \ldots (3.5) \end{aligned}$$

which is the same as that obtained by Hosoya[99] but now obtained far more easily.

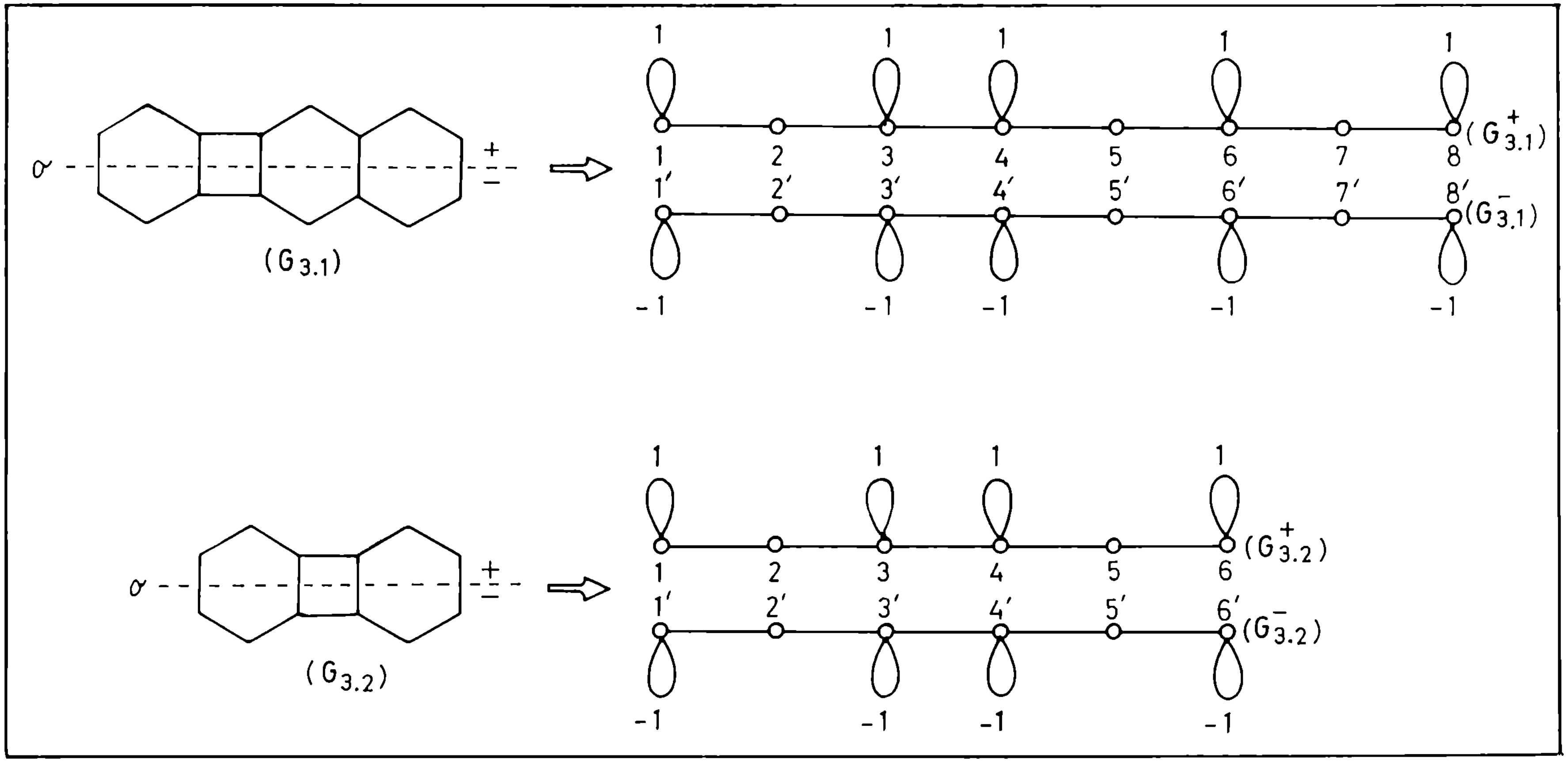

Fig. 3.1

Table 3.1. Building up of the coefficients of $G_{3.1}^{*}$

L_0 :	1								
$h_1\, L_0$:		1							
L_1 :	1	1							
$h_2\, L_1$:		0	0						
$-k^2_{1,2}\, L_0$:			−1						
L_2 :	1	1	−1						
$h_3\, L_2$:		1	1	−1					
$-k^2_{2,3}\, L_1$:			−1	−1					
L_3 :	1	2	−1	−2					
$h_4\, L_3$:		1	2	−1	−2				
$-k^2_{3,4}\, L_2$:			−1	−1	1				
L_4 :	1	3	0	−4	−1				
$h_5\, L_4$:		0	0	0	0	0			
$-k^2_{4,5}\, L_3$:			−1	−2	1	2			
L_5 :	1	3	−1	−6	0	2			
$h_6\, L_5$:		1	3	−1	−6	0	2		
$-k^2_{5,6}\, L_4$:			−1	−3	0	4	1		
L_6 :	1	4	1	−10	−6	6	3		
$h_7\, L_6$:		0	0	0	0	0	0	0	
$-k^2_{6,7}\, L_5$:			−1	−3	1	6	0	−2	
L_7 :	1	4	0	−13	−5	12	3	−2	
$h_8\, L_7$:		1	4	0	−13	−5	12	3	−2
$-k^2_{7,8}\, L_6$:			−1	−4	−1	10	6	−6	−3
L_8 :	1	5	3	−17	−19	17	21	−5	−5
		↓		↓		↓		↓	
$(-1)^r$:		(−)		(−)		(−)		(−)	

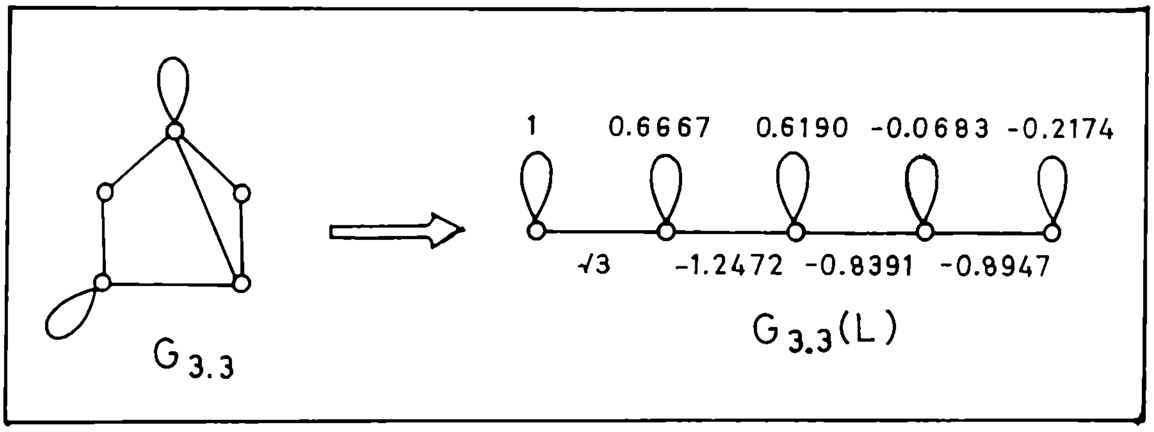

Fig. 3.2

Case II *Graphs that cannot be symmetry factorized*

Such a graph is $G_{3.3}$ (Fig.3.2), which was used in ref. 108 for illustration of the graph linearization algorithm using walks of unit length . The isospectral linear chain that can be obtained from $G_{3.3}$ through this algorithm is $G_{3.3}$ (L) (Fig.3.2). Using the present procedure the CP coefficients are built up in Table 3.2 . It is found that

$$P(G_{3.3} ; x) = P(G_{3.3} (L) ; x)$$
$$= x^5 - 2x^4 - 5x^3 + 5x^2 + 5x - 2 \quad . . . (3.6)$$

Table 3.2. Building up the CP coefficients of the nonsymmetric graph $G_{3.3}$

L_0 :	1					
$h_1 L_0$:		1				
L_1 :	1	1				
$h_2 L_1$:		0.6667	0.6667			
$-k^2_{1,2} L_0$:			-3			
L_2 :	1	1.6667	−2.3333			
$h_3 L_2$:		0.6190	1.0317	−1.4443		
$-k^2_{2,3} L_1$:			−1.5555	−1.5555		
L_3 :	1	2.2857	−2.8571	−2.9998		
$h_4 L_3$:		− 0.0683	−0.1561	+0.1951	+0.2049	
$-k^2_{3,4} L_2$:			−0.7041	− 1.1735	+1.6428	
L_4 :	1	2.2174	−3.7173	−3.9782	1.8477	
$h_5 L_4$:		−0.2174	−0.4821	+ 0.8081	+0.8649	− 0.4017
$-k^2_{4,5} L_3$:			−0.8005	−1.8297	+2.2871	+ 2.4013
L_5 :	1	2	-5	-5	5	2
		↓		↓		↓
$(-1)^r$:		(−)		(−)		(−)