Moments and characteristic polynomials for square lattice graphs

Hongxing Zhang and K. Balasubramanian*

Department of Chemistry, Arizona State University, Tempe, AZ 85287-1604, USA

The method of moments is used to derive closed analytical expressions for the characteristic polynomials of square lattice graphs. We obtain exact analytical formulae for three-dimensional cubic lattices, square lattices, tubular square lattices, and cylindrical square lattices containing any number of vertices.

1. Introduction

The computation of the characteristic polynomials of graphs has received considerable attention from mathematicians and chemists in the last two decades [1–41]. This is because not only are these polynomials important graph invariants, but they also have many applications in chemistry and physics, including chemical kinetics [40], quantum chemistry, dynamics of oscillatory reactions [32], lattice statistics [6,42,43], and the estimation of the stability of conjugated systems [24,30,31], formulation of the TEMO theory [40], electronic structure of organic polymers and periodic structures [3,9], etc.

Since Sachs published his famous theorem in 1963 [44], several approaches have been developed for the evaluation of the characteristic polynomials [16–31]. However, the practical computation of these polynomials remained as a very difficult problem until Balasubramanian programmed Frame's method [45,46] in 1984 [1]. Balasubramanian's program makes it possible for us to obtain the characteristic polynomials of arbitrary graphs, even ones containing several hundred vertices, by computer. However, it is important to derive analytical results or recursion formulae for the polynomials of homologous or special graphs, especially as the number of vertices approaches infinity. In fact, since the middle of the 1970s, Hosoya [16–22], Trinajstić [36], Gutman [23–25], Tang and Jiang [26–30], and other theoretical chemists have made significant efforts to develop such techniques. Several approaches such as the partition method, the contraction method and the operator method were developed to evaluate the characteristic polynomials and the eigenvalues (HMO energy levels) of chemical graphs [16–31]. Some of the results have been successfully used in a series of chemical homologous graphs.

*Camille and Henry Dreyfus Teacher–Scholar.

Recently, Jiang and Zhang [29,30,47–51] have developed the moment approach and the molecular fragment approach to rationalize systematically the aromaticity, total energy and chemical reactivities, as well as the characteristic polynomials of conjugated molecules and related graphs [51]. They expressed these polynomials in terms of the moments of graphs and in terms of fragments of bipartite graphs. One of the advantages of the moment method is that it provides not only a starting point for the computation of the characteristic polynomials, but also a convenient way to obtain the analytical or recursion formulae of the polynomials in terms of graph indices for homologous graphs.

In this paper, the moments of two- and three-dimensional square lattice graphs are expressed in terms of the moments of linear chains and single rings for planar square lattices, tubular square lattices, cubic square lattices and cylindrical square lattices, respectively. Thus, multi-dimensional problems are reduced to one-dimensional ones, which makes it possible to obtain the characteristic polynomials of such graphs even when they are very large. Furthermore, the moments of these graphs are expressed in terms of their graph size indices via the moment formula of linear chain and single rings. Subsequently, the characteristic polynomials are obtained from the moments.

2. Moment method for evaluation of characteristic polynomials

Several years ago, Jiang and Zhang [29,30,47–50] used the moment method in the context of chemical graph theory for rationalizing stability and reactivities of conjugated systems, although a similar moment method was used by Burdett and co-workers and others in extended Hückel theory [51,52]. One of the important results is that a set of formulae were obtained for expressing the characteristic polynomials in terms of the graph moments and in terms of molecular fragments for alternants [29,30]. These formulae can be conveniently used to evaluate the characteristic polynomials, in analytical or recursive form for homologous graphs. We now introduce the method briefly.

For any given graph G with N vertices, its characteristic polynomial $P_G(x)$ is defined as follows:

$$P_G(x) = |xI - A(G)| = x^N + a_1x^{N-1} + a_2x^{N-2} + \ldots + a_kx^{N-k} + \ldots + a_N, \quad (1)$$

where I is the identity matrix with dimension N, $A(G)$ is the adjacency matrix of graph G with its elements

$$A_{ij} = \begin{cases} 1, & \text{if vertices } i \text{ and } j \text{ are adjacent;} \\ 0, & \text{otherwise} \end{cases} \quad (2)$$

and a_k is the kth coefficient of the polynomial. What we need to do is to evaluate all the a_k's for a given graph.

Let $P_G(x) = 0$, with N real zero points $(x_1, x_2, \ldots, x_N)$, called the eigenvalues or the spectra of the graph G. The mth moment μ_m of graph G is defined as

$$\mu_m = x_1^m + x_2^m + \ldots + x_N^m = \sum_{i=1}^{N} x_i^m. \tag{3}$$

Obviously, an alternative definition of μ_m is

$$\mu_m = \mathrm{trace}(A^m). \tag{4}$$

Equation (4) can be taken as one of the algorithms for evaluating moments. It can be deduced from the relations between the coefficients of the polynomial and its zero points that

$$\begin{aligned} &\sum_{i=1}^{N} x_i = \mu_1 = -a_1, \\ &-2\sum_{i}^{N} \sum_{<j}^{N} x_i x_j = \mu_2 + a_1\mu_1 = -2a_2, \\ &3\sum_{i}^{N} \sum_{<j}^{N} \sum_{<k}^{N} x_i x_j x_k = \mu_3 + a_1\mu_2 + a_2\mu_1 = -3a_3, \\ &\qquad\qquad\qquad\vdots \end{aligned} \tag{5}$$

Finally, we can obtain

$$ka_k = -\sum_{i=1}^{k} a_{k-i}\mu_i. \tag{6}$$

Equation (6) is the recursion formula of the characteristic polynomial in terms of moments; it allows us to generate the kth coefficient a_k from $a_1, a_2, \ldots, a_{k-1}$ and $\mu_1, \mu_2, \ldots, \mu_k$. Generally, such a recursive expression can easily be programmed for computing any a_k via a_1 and moments by computer.

Now, let us recall Frame's recursion formula [2,3],

$$-a_k = \frac{1}{k}\,\mathrm{trace}(AA_{k-1}), \tag{7}$$

where A is the adjacency matrix, and A_{k-1} obeys the following equations:

$$\begin{aligned} A_0 &= I, \\ A_1 &= AA_0 + a_1 I, \\ A_2 &= AA_1 + a_2 I, \\ &\vdots \\ A_k &= AA_{k-1} + a_k I, \\ &\vdots \end{aligned} \tag{8}$$

Substituting eq. (8) into eq. (7), we have

$$-ka_k = \text{trace}(A^k + A^{k-1}a_1 + A^{k-2}a_2 + \ldots + A^1 a_{k-1})$$

$$= \mu_k + a_1\mu_{k-1} + a_2\mu_{k-2} + \ldots + a_{k-1}\mu_1.$$

This is eq. (6). So, the moment method used by Jiang and Tang subsequent to 1986 is equivalent to Frame's method used by Balasubramanian in 1984 and earlier by others in different contexts. From the induction of eq. (6), one can obtain [29]

$$a_k = \sum_{(m)} \prod_{l=1}^{k} \frac{1}{m_l!}\left(-\frac{\mu_l}{l}\right)^{m_l}, \tag{9}$$

where (m) signifies a set of non-negative integers $(m_1, m_2, \ldots, m_k)$ satisfying

$$k = 1m_1 + 2m_2 + \ldots + km_k = \sum_{l=1}^{k} lm_l.$$

Equation (9) clearly shows the relation between moments and characteristic polynomials. If the moments are known, we can calculate the characteristic polynomial from eq. (9). Since moments can be expressed in terms of the basic invariants of graphs, eq. (9) can be further transformed into a formula of the characteristic polynomial in terms of the basic invariants of graphs [28,29]. In this paper, we express the moments in terms of graph size indices for square lattice graphs, and obtain the characteristic polynomials from eq. (9). The advantage of the moment method, which we exploit fully in the present paper, is that it provides analytical formulas which can be extended to the limit when the number of vertices goes to infinity.

3. Moments of linear chains and single rings

As shown later, the moments of square lattice graphs are closely dependent on the moments of linear chains and single rings, so that we should obtain the moment formulae for these graphs. Many results, such as spectra and characteristic polynomials, have already been derived. Let us start from their graph spectra.

For any given linear chain and single ring with N vertices (see fig. 1), it is well known that from the Chebyshev polynomials or the symmetry method their eigenvalue spectra can be expressed as follows [31]:

$$x_p^{\mathrm{L}} = 2\cos\left(\frac{p\pi}{N+1}\right), \quad p = 1, 2, \ldots, N \text{ (for a linear chain)}, \tag{10}$$

$$x_p^{\mathrm{R}} = 2\cos\left(\frac{2p\pi}{N}\right), \quad p = 1, 2, \ldots, N \text{ (for a single ring)}, \tag{11}$$

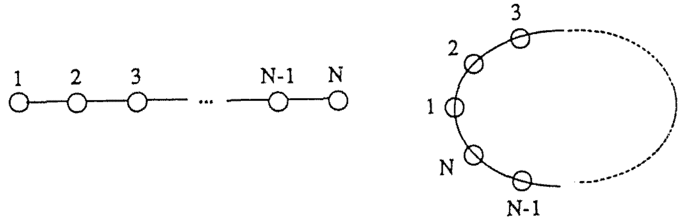


Fig. 1. Graphs of linear chain and single ring.

where x_p^{L} and x_p^{R} signify the pth eigenvalues of the linear chain and the single ring, respectively. Then from the moment definition, eq. (3), we have

$$\mu_m^{\mathrm{L}}(N) = 2^m \sum_{p=1}^{N} \cos^m\left(\frac{p\pi}{N+1}\right), \tag{12}$$

$$\mu_m^{\mathrm{R}}(N) = 2^m \sum_{p=1}^{N} \cos^m\left(\frac{2p\pi}{N}\right), \tag{13}$$

where $\mu_m^{\mathrm{L}}(N)$ and $\mu_m^{\mathrm{R}}(N)$ stand for mth moments of N-membered linear chains and single rings, respectively. Starting from eqs. (12) and (13) and using Euler's transformation, we can express moments of these graphs in terms of the graph size N and moment labels as follows:

(1) For an N-membered linear chain, it can be seen that

$$\begin{aligned} &\mu_{2n}^{\mathrm{L}}(N) = (N+1)C_{2n}^{n} - 2^{2n}, \\ &\mu_{2n+1}^{\mathrm{L}}(N) = 0, \end{aligned} \tag{14}$$

where C stands for the binomial coefficient. Generally, for any two non-negative integers a and b satisfying $a \geq b$, we have

$$C_a^b = \frac{a!}{b!(a-b)!}. \tag{15}$$

(2) Hence, for an N-membered single ring, we obtain

$$\begin{aligned} &\mu_{2n}^{\mathrm{R}}(2N) = 2NC_{2n}^{n} + 4N \sum_{m=1}^{[n/N]} C_{2n}^{n-Nm}, \\ &\mu_{2n+1}^{\mathrm{R}}(2N) = 0, \end{aligned} \tag{16}$$

$$\mu_{2n}^{\mathrm{R}}(2N+1) = (2N+1)C_{2n}^{n} + 2(2N+1) \sum_{m=1}^{[n/(2N+1)]} C_{2n}^{n-2mN-m}, \tag{17}$$

$$\mu^{R}_{2n+1}(2N+1) = 2(2N+1) \sum_{m=1}^{[(n+N+1)/(2N+1)]} C_{2n+1}^{n-2mN-m+N+1}, \tag{18}$$

where [ ] stands for the greatest integer containing the number within the square bracket.

4. Moments and characteristic polynomials of square lattices

As a set of important regular graphs in graph theory and statistical physics, square lattice graphs have received much attention either physically or mathematically in recent years [3,18,22,42,43]. They are the basis of two-dimensional Ising models and lattice gas statistics. In fact, the general dimer statistics of these graphs for partial coverings remains as yet unsolved. So, it is of interest to investigate the moments and characteristic polynomials of these graphs.

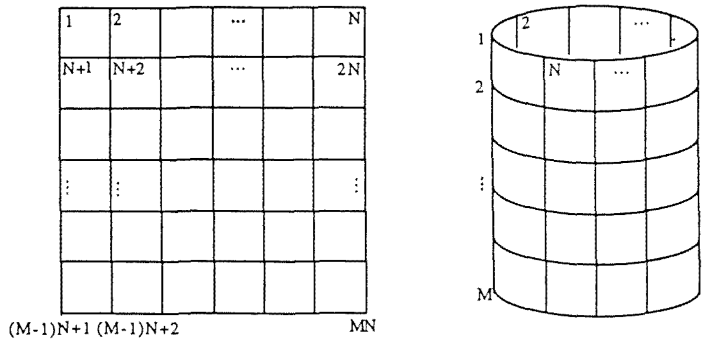
In this section, we consider two kinds of two-dimensional square lattice graphs, planar square lattices and tubular square lattices (see fig. 2), and two kinds of three-dimensional square lattice graphs, cubic square lattices and cylindric square lattices (see fig. 3). Here, we need pay attention only to planar square lattices; their results can be easily extended to the others. For any given planar square lattice with M rows and N columns, label its points as shown in fig. 2. Under this labelling, its adjacency matrix A is partitioned as follows:

$$A = \begin{bmatrix} A_N & I & & & \\ I & A_N & I & & \\ & I & \ddots & \ddots & \\ & & \ddots & A_N & I \\ & & & I & A_N \end{bmatrix}_{M\times M}, \tag{19}$$

where I is the N-dimensional identity matrix and A_N is exactly the adjacency matrix of an N-membered linear chain, i.e.

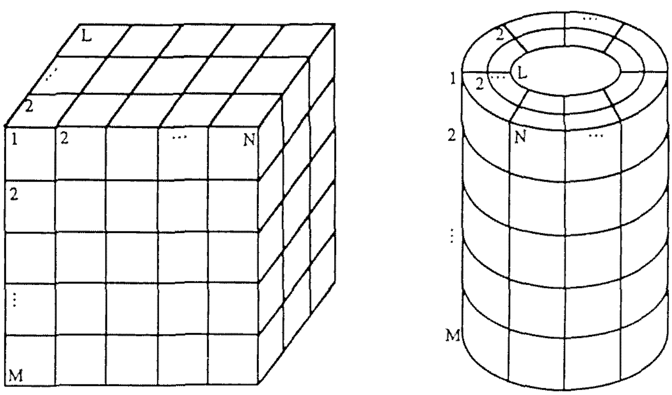
$$A_N = \begin{bmatrix} 0 & 1 & & \\ 1 & 0 & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & 0 \end{bmatrix}_{N\times N}, \tag{20}$$

$$I = \begin{bmatrix} 1 & & \\ & 1 & \\ & & \ddots & \\ & & & 1 \end{bmatrix}_{N\times N}, \tag{21}$$



Planar square lattice   Tubular square lattice

Fig. 2. Two-dimensional square lattice graphs.



Cubic square lattice   Cylindrical square lattice

Fig. 3. Three-dimensional square lattice graphs.

Let

$$B_M = \begin{bmatrix} A_N & & & \bigcirc \\ & A_N & & \\ & & \ddots & \\ \bigcirc & & & A_N \end{bmatrix}, \quad I_M = \begin{bmatrix} 0 & I & & \bigcirc \\ I & 0 & \ddots & \\ & \ddots & \ddots & I \\ \bigcirc & & I & 0 \end{bmatrix}, \tag{22}$$

then eq. (1) can be written as

$$A = B_M + I_M. \tag{23}$$

Since B_M and I_M are two commuting matrices, we obtain

$$A^{2n} = (B_M + I_M)^{2n} = \sum_{m'=0}^{2n} C_{2n}^{m'} B_M^{2n-m'} I_M^{m'}, \tag{24}$$

$$\mu_{2n}^{\mathrm{P}}(M \times N) = \mathrm{Tr}\,(A^{2n}) = \sum_{m'=0}^{2n} C_{2n}^{m'} \mathrm{Tr}\,(B_M^{2n-m'} I_M^{m'}), \tag{25}$$

where $\mu_{2n}^{\mathrm{P}}(M \times N)$ denotes the $2n$th moments of $M \times N$ planar square lattices. From (19) it can be seen that

$$B_M^{2n-m'} = \begin{bmatrix} A_N^{2n-m'} & & \mathbf{0} \\ & A_N^{2n-m'} & \\ \mathbf{0} & \ddots & \\ & & A_N^{2n-m'} \end{bmatrix}_{M\times M} . \tag{26}$$

When m' is an even number standing for $2m$, we obtain

$$I_M^{2m} = \begin{bmatrix} n_1 I & 0 & & \\ 0 & n_2 I & \ddots & \\ & \ddots & \ddots & 0 \\ & & 0 & n_M I \end{bmatrix}, \tag{27}$$

i.e. the diagonal is non-zero and other bands are alternatively zero, where $n_1 + n_2 + \ldots + n_M = \mu_{2m}^{\mathrm{L}}(M)$, i.e. the $2m$th moment of an M-membered linear chain. When m' is an odd number, $2m + 1$, we obtain

$$I_M^{2m+1} = \begin{bmatrix} 0 & m_1 I & & \\ m_1 I & 0 & \ddots & \\ & \ddots & \ddots & m_{M-1} I \\ & & m_{M-1} I & 0 \end{bmatrix}, \tag{28}$$

i.e. the diagonal is zero and the off-diagonal bands are non-zero alternatively. Using eqs. (23)–(26), we obtain

$$\mathrm{Tr}\,(B_M^{2n-2m} I_M^{2m}) = n_1 \mathrm{Tr}\,(A_N^{2n-2m}) + \ldots + n_M \mathrm{Tr}\,(A_N^{2n-2m})$$

$$= (n_1 + n_2 + \ldots + n_M)\mathrm{Tr}\,(A_N^{2n-m}), \tag{29}$$

$$\mathrm{Tr}\,(B_M^{2n-2m-1} I_M^{2m+1}) = 0. \tag{30}$$

Noticing that $n_1 + n_2 + \ldots + n_M = \mu^{\mathrm{L}}_{2m}(M)$, and using eq. (4), we have

$$\mathrm{Tr}\,(B_M^{2n-2m} I_M^{2m}) = \mu^{\mathrm{L}}_{2m}(M)\mu^{\mathrm{L}}_{2n-2m}(N). \tag{31}$$

Substituting eq. (28) into eq. (22), we obtain the final moment formula

$$\mu^{\mathrm{P}}_{2n}(M \times N) = \sum_{m=0}^{n} C_{2n}^{2m} \mu^{\mathrm{L}}_{2m}(M)\mu^{\mathrm{L}}_{2n-2m}(N),$$

$$\mu^{\mathrm{P}}_{2n+1}(M \times N) = 0. \tag{32}$$

Following the same procedure, we can obtain the moment formulae of the tubular, cubic and cylindric square lattices as follows.

For the tubular square lattice, spanned by an M-membered linear chain and an N-membered single ring, we obtain

$$\mu^{\mathrm{T}}_{2n}(M \times N) = \sum_{m=0}^{n} C_{2n}^{2m} \mu^{\mathrm{L}}_{2m}(M)\mu^{\mathrm{R}}_{2n-2m}(N), \tag{33}$$

$$\mu^{\mathrm{T}}_{2n+1}(M \times N) = \sum_{m=0}^{n} C_{2n+1}^{2m} \mu^{\mathrm{L}}_{2m}(M)\mu^{\mathrm{R}}_{2n+1-2m}(N). \tag{34}$$

For the cubic square lattice spanned by three M-, N-, L-membered linear chains, it can be seen that

$$\mu^{\mathrm{Cb}}_{2n}(M \times N) = \sum_{m=0}^{n} \sum_{l=0}^{m} C_{2n}^{2m} C_{2m}^{2l} \mu^{\mathrm{L}}_{2l}(L)\mu^{\mathrm{L}}_{2m-2l}(M)\mu^{\mathrm{R}}_{2n-2m}(N),$$

$$\mu^{\mathrm{Cb}}_{2n+1}(M \times N \times L) = 0. \tag{35}$$

For the cylindrical square lattice spanned by M- and L-membered linear chains and an N-membered single ring, we obtain

$$\mu^{\mathrm{Cl}}_{2n}(M \times N \times L) = \sum_{m=0}^{n} \sum_{l=0}^{m} C_{2n}^{2m} C_{2m}^{2l} \mu^{\mathrm{L}}_{2l}(L)\mu^{\mathrm{L}}_{2m-2l}(M)\mu^{\mathrm{R}}_{2n-2m}(N), \tag{36}$$

$$\mu^{\mathrm{Cl}}_{2n+1}(M \times N \times L) = \sum_{m=0}^{n} \sum_{l=0}^{m} C_{2n+1}^{2m} C_{2m}^{2l} \mu^{\mathrm{L}}_{2l}(L)\mu^{\mathrm{L}}_{2m-2l}(M)\mu^{\mathrm{R}}_{2n+1-2m}(N). \tag{37}$$

Equations (32)–(37) successfully express the moments of two- and three-dimensional square lattices in terms of moments of chains and rings. It is obvious that this set of formulae simplifies greatly the evaluation of moments for lattice graphs. Substituting eqs. (14), (16)–(18) into eqs. (32)–(37), we can derive the moments formulae of two- and three-dimensional square lattices in terms of their graph size indices.

For the planar square lattice spanned by M- and N-membered linear chains, we obtain

$$\mu_{2n}^{\mathrm{P}}(M \times N) = \sum_{m=0}^{n} P(M, N, m),$$
$$\mu_{2n+1}^{\mathrm{P}}(M \times N) = 0, \tag{38}$$

where

$$P(M, N, m) = C_{2n}^{2m}[(M+1)C_{2m}^{m} - 2^{2m}][(N+1)C_{2n-2m}^{n-m} - 2^{2n-2m}]. \tag{39}$$

For the tubular square lattice spanned by an M-membered linear chain and N_{R}-membered single ring ($N_{\mathrm{R}} = 2N$ or $2N+1$), we get

$$\mu_{2n}^{\mathrm{T}}(M \times 2N) = \sum_{m=0}^{n} T_1(M, N, m),$$
$$\mu_{2n+1}^{\mathrm{T}}(M \times 2N) = 0, \tag{40}$$

$$\mu_{2n}^{\mathrm{T}}[M \times (2N+1)] = \sum_{m=0}^{n} T_2(M, N, m), \tag{41}$$

$$\mu_{2n+1}^{\mathrm{T}}[M \times (2N+1)] = \sum_{m=0}^{n} T_3(M, N, m), \tag{42}$$

where

$$T_1(M, N, m) = C_{2n}^{2m}[(M+1)C_{2m}^{m} - 2^{2m}]\{2NC_{2n-2m}^{n-m} + 4N \sum_{q=1}^{[(n-m)/N]} C_{2n-2m}^{n-m-Nq}\}, \tag{43}$$

$$T_2(M, N, m) = C_{2n}^{2m}[(M+1)C_{2m}^{m} - 2^{2m}]$$
$$\times \{(2N+1)C_{2n-2m}^{n-m} + 2(2N+1) \sum_{q=1}^{[(n-m)/(2N+1)]} C_{2n-2m}^{n-m-N-q}\}, \tag{44}$$

$$T_3(M, N, m) = 2(2N+1)C_{2n}^{2m}[(M+1)C_{2m}^{m} - 2^{2m}]$$
$$\times \sum_{q=1}^{[(n-m+N+1)/(2N+1)]} C_{2n-2m+1}^{n-m-2qN-q+N+1}. \tag{45}$$

For the cubic square lattice spanned by M-, N-, and L-membered linear chains, we obtain

$$\mu_{2n}^{\mathrm{Cb}}(M\times N\times L)=\sum_{m=0}^{n}\mathrm{Cb}(M,N,L,m),$$
$$\mu_{2n+1}^{\mathrm{Cb}}(M\times N\times L)=0, \tag{46}$$

where

$$\mathrm{Cb}(M,N,L,m)=C_{2n}^{2m}[(N+1)C_{2n-2m}^{n-m}-2^{2n-2m}]$$
$$\times\sum_{l=0}^{m}C_{2m}^{2l}[(L+1)C_{2l}^{l}-2^{2l}][(M+1)C_{2m-2l}^{m-l}-2^{2m-2l}]. \tag{47}$$

For the cylindrical square lattice spanned by L- and M-membered linear chains and an N_{R}-membered single ring ($N_{\mathrm{R}}=2N$ or $2N+1$), we obtain

$$\mu_{2n}^{\mathrm{Cl}}(M\times 2N\times L)=\sum_{m=0}^{n}\mathrm{Cl}_1(M,N,L,m),$$
$$\mu_{2n+1}^{\mathrm{Cl}}(M\times 2N\times L)=0, \tag{48}$$

$$\mu_{2n}^{\mathrm{Cl}}[M\times(2N+1)\times L]=\sum_{m=0}^{n}\mathrm{Cl}_2(M,N,L,m), \tag{49}$$

$$\mu_{2n+1}^{\mathrm{Cl}}[M\times(2N+1)\times L]=\sum_{m=0}^{n}\mathrm{Cl}_3(M,N,L,m), \tag{50}$$

where

$$\mathrm{Cl}_1(M,N,L,m)=C_{2n}^{2m}\{2NC_{2n-2m}^{n-m}+4N\sum_{q=1}^{[(n-m)/N]}C_{2n-2m}^{n-m-Nq}\}$$
$$\times\sum_{l=0}^{m}\mathrm{Cl}_{2m}^{2l}[(L+1)C_{2l}^{l}-2^{2l}][(M+1)C_{2m-2l}^{m-l}-2^{2m-2l}], \tag{51}$$

$$\mathrm{Cl}_2(M,N,L,m)=C_{2n}^{2m}\{(2N+1)C_{2n-2m}^{n-m}+2(2N+1)\sum_{q=1}^{[(n-m)/(2N+1)]}C_{2n-2m}^{n-m-2qN-q}\}$$
$$\times\sum_{l=0}^{m}\mathrm{Cl}_{2m}^{2l}[(L+1)C_{2l}^{l}-2^{2l}][(M+1)C_{2m-2l}^{m-l}-2^{2m-2l}], \tag{52}$$

$$\mathrm{Cl}_3(M,N,L,m) = C_{2n+1}^{2m}(4N+2)\sum_{q=1}^{[(n-m+N+1)/(2N+1)]} C_{2n-2m+1}^{n-m-2qN-q+N+1}$$
$$\times\sum_{l=0}^{m}\mathrm{Cl}_{2m}^{2l}[(L+1)C_{2l}^{l}-2^{2l}][(M+1)C_{2m-2l}^{m-l}-2^{2m-2l}]. \qquad (53)$$

Equations (38)–(53) are the moment formulae of two- and three-dimensional square lattices in terms of their graph size indices L, M and N. On substituting them into eq. (6) or eq. (9), the characteristic polynomials can be obtained. For planar square lattices

$$a_{2k}(M\times N) = \sum_{(m_1,m_2,\ldots,m_k)}\prod_{l-1}^{k}\frac{1}{m_l!}\left[-\frac{1}{2l}\sum_{m=0}^{l}P(M,N,m)\right]^{m_l}, \qquad (54)$$

where $\sum_{l=1}^{k} lm_l = k$;

$a_{2k+1}(M\times N) = 0.$

For tabular square lattices

$$a_{2k}(M\times 2N) = \sum_{(m_1,m_2,\ldots,m_k)}\prod_{l-1}^{k}\frac{1}{m_l!}\left[-\frac{1}{2l}\sum_{m=0}^{l}T_1(M,N,m)\right]^{m_l}, \qquad (55)$$

where $\sum_{l=1}^{k} lm_l = k$;

$a_{2k+1}(M\times 2N) = 0;$

$$a_{2k}[M\times(2N+1)] = \sum_{(m_1,m_2,\ldots,m_{2k})}\prod_{\text{even } l}^{2k}\frac{1}{m_l!}\left[-\frac{1}{l}\sum_{m=0}^{l/2}T_2(M,N,m)\right]^{m_l}$$
$$\times\prod_{\text{odd } l}^{2k-1}\frac{1}{m_l!}\left[-\frac{1}{l}\sum_{m=0}^{(l-1)/2}T_3(M,N,m)\right]^{m_l}, \qquad (56)$$

where $\sum_{l=1}^{2k} lm_l = 2k$;

$$a_{2k+1}[M \times (2N+1)] = \sum_{(m_1, m_2, \ldots, m_{2k+1})} \prod_{\text{even } l}^{2k} \frac{1}{m_l!} \left[-\frac{1}{l} \sum_{m=0}^{l/2} T_2(M, N, m) \right]^{m_l}$$

$$\times \prod_{\text{odd } l}^{2k+1} \frac{1}{m_l!} \left[-\frac{1}{l} \sum_{m=0}^{(l-1)/2} T_3(M, N, m) \right]^{m_l}, \tag{57}$$

where $\sum_{l=1}^{2k+1} l m_l = 2k+1.$

For cubic square lattices

$$a_{2k}[M \times N \times L] = \sum_{(m_1, m_2, \ldots, m_k)} \prod_{l=1}^{k} \frac{1}{m_l!} \left[-\frac{1}{2l} \sum_{m=0}^{l} \mathrm{Cb}(M, L, m) \right]^{m_l}, \tag{58}$$

where $\sum_{l=1}^{k} l m_k = k;$

$a_{2k+1}[M \times N \times L] = 0.$

For cylindrical square lattices

$$a_{2k}[M \times 2N \times L] = \sum_{(m_1, m_2, \ldots, m_k)} \prod_{l=1}^{k} \frac{1}{m_l!} \left[-\frac{1}{2l} \sum_{m=0}^{l} \mathrm{Cl}_1(M, L, m) \right]^{m_l}, \tag{59}$$

where $\sum_{l=1}^{k} l m_l = k;$

$a_{2k+1}[M \times 2N \times L] = 0;$

$$a_{2k}[M \times (2N+1) \times L] = \sum_{(m_1, m_2, \ldots, m_{2k})} \prod_{\text{even } l}^{2k} \frac{1}{m_l!} \left[-\frac{1}{l} \sum_{m=0}^{l/2} \mathrm{Cl}_2(M, N, L, m) \right]^{m_l}$$

$$\times \prod_{\text{odd } l}^{2k-1} \frac{1}{m_l!} \left[-\frac{1}{l} \sum_{m=0}^{(l-1)/2} \mathrm{Cl}_3(M, N, L, m) \right]^{m_l}, \tag{60}$$

where $\sum_{l=1}^{2k} l m_l = 2k;$

$$a_{2k+1}[M\times(2N+1)\times L]=\sum_{(m_1,m_2,\ldots,m_{2k+1})}\prod_{\text{even }l}^{2k}\frac{1}{m_l!}\left[-\frac{1}{l}\sum_{m=0}^{l/2}\text{Cl}_2(M,N,L,m)\right]^{m_l}$$

$$\times\prod_{\text{odd }l}^{2k+1}\frac{1}{m_l!}\left[-\frac{1}{l}\sum_{m=0}^{(l-1)/2}\text{Cl}_3(M,N,L,m)\right]^{m_l}, \qquad (61)$$

where $\sum_{l=1}^{2k+1} lm_l = 2k+1.$

Equations (54)–(61) are the analytical formulae of characteristic polynomials for square lattice graphs obtained from the moment method, which allows us to evaluate the polynomials of these graphs even as the graph indices M, N, and L tend to infinite. This indicates that the moment method is also effective for computing the characteristic polynomial and especially in dering the analytical or recursion formulae for homologous series. An open problem now is how to extend this method to other systems, for example an infinite honeycomb lattice graph.

In 1983, Hosoya and Ohkami [19] developed a systematic approach, called the operator method, for evaluating various kinds of polynomials, such as the characteristic polynomial, the matching polynomial, the king polynomial, etc., of homologous graphs. Since then, Hosoya and co-workers have applied this approach to a series of homologous graphs and obtained many recursion formulae [19–22]. Essentially, the operator method is based on the partitioning technique, so that its use depends on how many kinds of graphs are formed when we delete some edges in the graph considered. Generally, if the partitioning method yields more than four graphs, it seems to be difficult to obtain the eigenvalues of the operator determinant. In two- or three-dimensional homologous graphs there are, respectively, two or three graph size indices, such as M, N, L in square lattice graphs. The operator method can work only when one of the indices tends to infinity, which means that the method is more effective for one-dimensional problems rather than two- or three-dimensional ones. However, the operator method is universally applicable to all kinds of polynomials, while the moment method is not. For example, the moment method is difficult to use for matching polynomials because it is difficult to obtain "matching moments".

Acknowledgement

One of the authors (HZ) thanks Professor Yuansheng Jiang for useful discussions on the moment method, and the Institute of Theoretical Chemistry, Jilin University, Changchun, PR China, for providing a leave which made this joint study possible.

References

[1] K. Balasubramanian, Int. J. Quant. Chem. 21(1982)581.
[2] K. Balasubramanian, Theor. Chim. Acta 65(1984)49.
[3] K. Balasubramanian, J. Comput. Chem. 3(1984)357; 6(1985)656; 11(1990)829.
[4] K. Balasubramanian, Comput. Chem. 9(1985)43.
[5] K. Balasubramanian, Chem. Rev. 88(1985)559.
[6] K. Balasubramanian, J. Math. Chem. 2(1988)69; 4(1990)89.
[7] K. Balasubramanian, in: *Studies in Physical and Theoretical Chemistry*, ed. R.B. King and D.H. Rouvray (Elsevier, Amsterdam, 1983) pp. 243–251.
[8] K. Balasubramanian, in: *Mathematical and Computational Concepts in Chemistry*, ed. N. Trinajstić (Ellis Horwood, Chichester, 1986) pp. 20–33.
[9] K. Balasubramanian, in: *Chemical Applications of Graph Theory and Topology*, ed. R.B. King and D.H. Rouvray (Elsevier, Amsterdam, 1987) p. 514.
[10] M. Randić, J. Comput. Chem. 1(1980)386.
[11] M. Randić, Theor. Chim. Acta 62(1983)485.
[12] M. Randić, J. Math. Chem. 1(1987)145.
[13] M. Randić, SIAM J. Algebraic Discr. Meth. 6(1985)145.
[14] K. Balasubramanian and M. Randić, Theor. Chim. Acta 61(1982)307.
[15] K. Balasubramanian and M. Randić, Int. J. Quant. Chem. 28(1985)481.
[16] H. Hosoya, Bull. Chem. Soc. Japan 49(1971)2332; 52(1979)1624.
[17] H. Hosoya, Theor. Chim. Acta 25(1972)215.
[18] H. Hosoya, J. Math. Phys. 18(1977)1485.
[19] H. Hosoya and N. Ohkami, J. Comput. Chem. 4(1983)585.
[20] H. Hosoya and M. Randić, Theor. Chim. Acta 63(1983)473.
[21] M. Randić, H. Hosoya and O.E. Polansky, J. Comput. Chem. 10(1989)683.
[22] H. Hosoya, J. Math. Chem. 3(1989)383; 7(1990)289.
[23] I. Gutman, Theor. Chim. 45(1977)79.
[24] I. Gutman and O.E. Polansky, Theor. Chim. Acta 60(1982)203.
[25] I. Gutman, J. Math. Chem. 1(1987)123.
[26] A.C. Tang and Y.S. Kiang, Sci. Sinica 1(1976)448.
[27] A.C. Tang and Y.S. Kiang, Sci. Sinica 3(1977)218.
[28] Y.S. Kiang, Int. J. Quant. Chem. 18(1980)331; S15(1981)293.
[29] Y.S. Kiang and A.C. Tang, Int. J. Quant. Chem. 29(1986)229.
[30] Y.S. Jiang and H. Zhang, J. Math. Chem. 3(1989)357.
[31] A.C. Tang, Y.S. Kiang, G.S. Yan and S.S. Dai, *Molecular Graphical Orbital* (Science Press, Beijing, 1986).
[32] D.M. Cvetković, M. Doob and H. Sachs, *Spectra of Graphs* (Academic Press, New York, 1980).
[33] R.B. King, Theor. Chim. Acta 44(1977)223; 56(1980)269.
[34] D.H. Rouvray, in: *Chemical Applications of Graph Theory*, ed. A.T. Balaban (Academic Press, New York, 1976).
[35] R.B. Mallion and D.H. Rouvray, Mol. Phys. 36(1978)125.
[36] N. Trinajstić, *Chemical Graph Theory*, Vol. 1 (CRC Press, Boca Raton, 1983).
[37] E.C. Kirby, J. Math. Chem. 1(1987)175.
[38] S. El-Basil, Theor. Chim. Acta 65(1985)199.
[39] R. Barakat, Theor. Chim. Acta 69(1985)135.
[40] L. Glass, J. Chem. Phys. 63(1975)1325.
[41] O.E. Polansky and M. Zandler, J. Mol. Struct. 84(1982)361.
[42] E. Montroll, in: *Applied Combinatorial Mathematics*, ed. E.F. Beckenbach (Wiley, New York, 1964).

[43] J.E. Kilpatrick, Adv. Chem. Phys. 20(1971)39.
[44] H. Sachs, Publ. Math. Debrencen 11(1963)119.
[45] J.S. Frame, A simle recursion formula for inverting a matrix, paper presented to the American Mathematical Society at Boulder, CO, September 1, 1949 (as referred to in ref. [44]).
[46] P.S. Dwyer, *Linear Computation* (Wiley, New York, 1951) p. 225–235.
[47] Y. Jiang and H. Zhang, Sci. Sinica (Chinese) 2(1988)122.
[48] H. Zhang and Y. Jiang, Sci. Sinica (Chinese) 6(1988)565.
[49] Y. Jiang and H. Zhang, Theor. Chim. Acta 75(1989)279.
[50] Y. Jiang, H. Zhu and H. Zhang, Chem. Phys. Lett. 159(1989)159.
[51] Y. Jiang, A. Tang and R. Hoffman, Theor. Chim. Acta 66(1985)853.
[52] J.K. Burdett and S. Lee, J. Am. Chem. Soc. 107(1985)3050, 3063, 3083;
J.K. Burdett, in: *Graph Theory and Topology in Chemistry*, ed. R.B. King and D.H. Rouvray (Elsevier, Amsterdam, 1987) pp. 202–324.