Chapter 11
Spectral Properties of Graphs

11.1 Introduction

In this chapter, we look at the properties of graphs from our knowledge of their eigenvalues. The set of eigenvalues of a graph G is known as the *spectrum* of G and denoted by $Sp(G)$. We compute the spectra of some well-known families of graphs—the family of complete graphs, the family of cycles etc. We present Sachs' theorem on the spectrum of the line graph of a regular graph. We also obtain the spectra of product graphs—Cartesian product, direct product, and strong product. We introduce Cayley graphs and Ramanujan graphs and highlight their importance. Finally, as an application of graph spectra to chemistry, we discuss the "*energy of a graph*"—a graph invariant that is widely studied these days. All graphs considered in this chapter are finite, undirected, and simple.

11.2 The Spectrum of a Graph

Let G be a graph of order n with vertex set $V = \{v_1, \ldots, v_n\}$. The *adjacency matrix* of G (with respect to this labeling of V) is the n by n matrix $A = (a_{ij})$, where

$$a_{ij} = \begin{cases} 1 & \text{if } v_i \text{ is adjacent to } v_j \text{ in } G \\ 0 & \text{otherwise.} \end{cases}$$

Thus A is a real symmetric matrix of order n. Hence,

(i) The spectrum of A, that is, the set of its eigenvalues is real.
(ii) $\mathbb{R}^n$ has an orthonormal basis of eigenvectors of A.
(iii) The sum of the entries of the ith row (column) of A is $d(v_i)$ in G.

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The spectrum of A is called the *spectrum* of G and denoted by $Sp(G)$. We note that $Sp(G)$, as defined above, depends on the labeling of the vertex set V of G. We now show that it is independent of the labeling of G. Suppose we consider a new labeling of V. Let A' be the adjacency matrix of G with respect to this labeling. The new labeling can be obtained from the original labeling by means of a permutation π of $V(G)$. Any such permutation can be effected by means of a *permutation matrix* P of order n (got by permuting the rows of I_n, the identity matrix of order n). (For example, if $n = 3$, the permutation matrix $P = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$ takes v_1, v_2, v_3 to v_3, v_1, v_2 respectively since $(1\ 2\ 3)\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = (3\ 1\ 2)$.

Let $P = (p_{ij})$. Now given the new labeling of V, that is, given the permutation π on $\{1, 2, \ldots, n\}$, and the vertices v_i and v_j, there exist unique α_0 and β_0, such that $\pi(i) = \alpha_0$ and $\pi(j) = \beta_0$ or equivalently $p_{\alpha_0 i} = 1$ and $p_{\beta_0 j} = 1$, while for $\alpha \neq \alpha_0$ and $\beta \neq \beta_0$, $p_{\alpha i} = 0 = p_{\beta j}$. Thus, the (α_0, β_0)th entry of the matrix $A' = PAP^{-1} = PAP^{\mathrm{T}}$ (where P^{T} stands for the transpose of P) is

$$\sum_{k,l=1}^{n} p_{\alpha_0 k} a_{kl} p_{\beta_0 l} = a_{ij}\,.$$

Hence, $v_{\alpha_0} v_{\beta_0} \in E(G)$ if and only if $v_i v_j \in E(G)$. This proves that the adjacency matrix of the same graph with respect to two different labelings are similar matrices. But then similar matrices have the same spectra. □

We usually arrange the eigenvalues of G in their nondecreasing order: $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. If $\lambda_1, \ldots, \lambda_s$ are the distinct eigenvalues of G, and if m_i is the multiplicity of λ_i as an eigenvalue of G, we write

$$Sp(G) = \begin{pmatrix} \lambda_1 & \lambda_2 & \ldots & \lambda_s \\ m_1 & m_2 & \ldots & m_s \end{pmatrix}.$$

Definition 11.2.1. The *characteristic polynomial* of G is the characteristic polynomial of the adjacency matrix of G with respect to some labeling of G. It is denoted by $\chi(G;\lambda)$.

Hence, $\chi(G;\lambda) = \det(xI - A) = \det(P(xI - A)P^{-1}) = \det(xI - PAP^{-1})$ for any permutation matrix of P, and hence $\chi(G;\lambda)$ is also independent of the labeling of $V(G)$.

Definition 11.2.2. A *circulant of order n* is a square matrix of order n in which all the rows are obtainable by successive cyclic shifts of one of its rows (usually taken as the first row).

For example, the circulant with first row $(a_1\ a_2\ a_3)$ is the matrix $\begin{pmatrix} a_1 & a_2 & a_3 \\ a_3 & a_1 & a_2 \\ a_2 & a_3 & a_1 \end{pmatrix}$.

Lemma 11.2.3. *Let A be a circulant matrix of order n with first row* $(a_1\, a_2 \dots a_n)$. *Then* $Sp(A) = \{a_1 + a_2\omega + \cdots + a_n\omega^{n-1} : \omega = \text{an nth root of unity}\} = \{a_1 + \zeta^r + \zeta^{2r} + \cdots + \zeta^{(n-1)r},\ 0 \le r \le n-1 \text{ and } \zeta = \text{a primitive nth root of unity}\}$

Proof. The characteristic polynomial of A is the determinant $D = \det(xI - A)$. Hence,

$$D = \begin{vmatrix} x-a_1 & -a_2 & \dots & -a_n \\ -a_n & x-a_1 & \dots & -a_{n-1} \\ \vdots & \vdots & & \vdots \\ -a_2 & -a_3 & \dots & x-a_1 \end{vmatrix}.$$

Let C_i denote the ith column of D, $1 \le i \le n$, and ω, an nth root of unity. Replace C_1 by $C_1 + C_2\omega + \cdots + C_n\omega^{n-1}$. This does not change D. Let $\lambda_\omega = a_1 + a_2\omega + \cdots + a_n\omega^{n-1}$. Then the new first column of D is $(x - \lambda_\omega, \omega(x - \lambda_\omega), \dots, \omega^{n-1}(x - \lambda_\omega))^{\mathrm{T}}$, and hence $x - \lambda_\omega$ is a factor of D. This gives $D = \prod_{\omega : \omega^n = 1} (x - \lambda_\omega)$, and $Sp(A) = \{\lambda_\omega : \omega^n = 1\}$. □

11.3 Spectrum of the Complete Graph K_n

For K_n, the adjacency matrix A is given by $A = \begin{pmatrix} 0 & 1 & 1 & \dots & 1 \\ 1 & 0 & 1 & \dots & 1 \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & 1 & 1 & \dots & 0 \end{pmatrix}$, and so by Lemma 11.2.3,

$$\lambda_\omega = \omega + \omega^2 + \cdots + \omega^{n-1}$$
$$= \begin{cases} n-1 & \text{if } \omega = 1 \\ -1 & \text{if } \omega \ne 1. \end{cases}$$

Hence, $Sp(K_n) = \begin{pmatrix} n-1 & -1 \\ 1 & n-1 \end{pmatrix}$.

11.4 Spectrum of the Cycle C_n

Label the vertices of C_n as $0, 1, 2, \dots, n-1$ in this order. Then i is adjacent to $i \pm 1 (\bmod n)$. Hence,

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & 1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & \dots & 1 & 0 \end{bmatrix}$$

is the circulant with the first row (0 1 0 ... 0 1). Again, by Lemma 11.2.3, $Sp(C_n) = \{\omega^r + \omega^{r(n-1)} : 0 \leq r \leq n-1$, where ω is a primitive nth root of unity$\}$. Taking $\omega = \cos\frac{2\pi}{n} + i\sin\frac{2\pi}{n}$, we get $\lambda_r = \omega^r + \omega^{r(n-1)} = (\cos\frac{2\pi r}{n} + i\sin\frac{2\pi r}{n}) + (\cos\frac{2\pi r(n-1)}{n} + i\sin\frac{2\pi r(n-1)}{n})$. This simplifies to the following:

(i) If n is odd, $Sp(C_n) = \begin{pmatrix} 2 & 2\cos\frac{2\pi}{n} & \dots & 2\cos\frac{(n-1)\pi}{n} \\ 1 & 2 & \dots & 2 \end{pmatrix}$.

(ii) If n is even, $Sp(C_n) = \begin{pmatrix} 2 & 2\cos\frac{2\pi}{n} & \dots & 2\cos\frac{(n-1)\pi}{n} & -2 \\ 1 & 2 & \dots & 2 & 1 \end{pmatrix}$.

11.4.1 *Coefficients of the Characteristic Polynomial*

Let G be a connected graph on n vertices, and let $\chi(G;x) = \det(xI_n - A) = x^n + a_1x^{n-1} + a_2x^{n-2} + \dots + a_n$ be the characteristic polynomial of G. It is easy to check that $(-1)^r a_r =$ sum of the principal minors of A of order r. (Recall that a principal minor of order r of A is the determinant minor of A common to the same set of r rows and columns.)

Lemma 11.4.1. *Let G be a graph of order n and size m, and let $\chi(G;x) = x^n + a_1x^{n-1} + a_2x^{n-2} + \dots + a_n$ be the characteristic polynomial of A. Then*

(i) $a_1 = 0$
(ii) $a_2 = -m$
(iii) $a_3 = -$ *(twice the number of triangles in G)*

Proof. (i) Follows from the fact that all the entries of the principal diagonal of A are zero.

(ii) A nonvanishing principal minor of order 2 of A is of the form $\begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}$ and its value is -1. Since any 1 in A corresponds to an edge of G, we get (ii).

(iii) A nontrivial principal minor of order 3 of A can be one of the following three types:

$$\begin{vmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{vmatrix}, \begin{vmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{vmatrix}, \begin{vmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix}.$$

Of these, only the last determinant is nonvanishing. Its value is 2 and corresponds to a triangle in G. This proves (iii). □

11.5 The Spectra of Regular Graphs

In this section, we look at the spectra of some regular graphs.

Theorem 11.5.1. *Let G be a k-regular graph of order n. Then*

(i) *k is an eigenvalue of G.*
(ii) *If G is connected, every eigenvector corresponding to the eigenvalue k is a multiple of $\mathbf{1}$, (the all 1-column vector of length n) and the multiplicity of k as an eigenvalue of G is one.*
(iii) *For any eigenvalue λ of G, $|\lambda| \leq k$. (Hence $Sp(G) \subset [-k, k]$).*

Proof. (i) We have $A\mathbf{1} = k\mathbf{1}$, and hence k is an eigenvalue of A.

(ii) Let $\mathbf{x} = (x_1, \ldots, x_n)^{\mathrm{T}}$ be any eigenvector of A corresponding to the eigenvalue k so that $A\mathbf{x} = k\mathbf{x}$. We may suppose that $\mathbf{x}$ has a positive entry (otherwise, take $-\mathbf{x}$ in place of $\mathbf{x}$) and that x_j is the largest positive entry in $\mathbf{x}$. Let $v_{i_1}, v_{i_2}, \ldots, v_{i_k}$ be the k neighbors of v_j in G. Taking the inner product of the jth row of A with $\mathbf{x}$, we get $x_{i_1} + x_{i_2} + \cdots + x_{i_k} = kx_j$. This gives, by the choice of x_j, $x_{i_1} = x_{i_2} = \ldots = x_{i_k} = x_j$.

Now start at $v_{i_1}, v_{i_2}, \ldots, v_{i_k}$ in succession and look at their neighbors in G. As before, the entries x_p in $\mathbf{x}$ corresponding to these neighbors must all be equal to x_j. As G is connected, all the vertices of G are reachable in this way step by step. Hence $\mathbf{x} = x_j(1, 1, \ldots, 1)^{\mathrm{T}}$, and every eigenvector $\mathbf{x}$ of A corresponding to the eigenvalue k is a multiple of $\mathbf{1}$. Thus, the space of eigenvectors of A corresponding to the eigenvalue k is one-dimensional, and therefore, the multiplicity of k as an eigenvalue of G is 1.

(iii) The proof is similar to (ii). If $A\mathbf{y} = \lambda\mathbf{y}$, $\mathbf{y} \neq \mathbf{0}$, and if y_j is the entry in $\mathbf{y}$ with the largest absolute value, we see that the equation $\sum_{p=1}^{k} y_{i_p} = \lambda y_j$ implies that $|\lambda||y_j| = |\lambda y_j| = \left| \sum_{p=1}^{k} y_{i_p} \right| \leq \sum_{p=1}^{k} |y_{i_p}| \leq k|y_j|$. Thus, $|\lambda| \leq k$. □

Corollary 11.5.2. *If Δ denotes the maximum degree of G, then for any eigenvalue λ of G, $|\lambda| \leq \Delta$.*

Proof. Considering a vertex v_j of maximum degree Δ, and imitating the proof of (iii) above, we get $|\lambda||y_j| \leq \Delta|y_j|$. □

11.5.1 The Spectrum of the Complement of a Regular Graph

Theorem 11.5.3. *Let G be a k-regular connected graph of order n with spectrum $\begin{pmatrix} k & \lambda_2 & \lambda_3 & \ldots & \lambda_s \\ 1 & m_2 & m_3 & \ldots & m_s \end{pmatrix}$. Then the spectrum of G^c, the complement of G, is given by $Sp(G^c) = \begin{pmatrix} n-1-k & -\lambda_2 - 1 & -\lambda_3 - 1 & \ldots & -\lambda_s - 1 \\ 1 & m_2 & m_3 & \ldots & m_s \end{pmatrix}$.*

Proof. As G is k-regular, G^c is $n-1-k$ regular, and hence by Theorem 11.5.1, $n-1-k$ is an eigenvalue of G^c. Further, the adjacency matrix of G^c is $A^c = J - I - A$, where J is the all-1 matrix of order n, I is the identity matrix of order n, and A is the adjacency matrix of G. If $\chi(\lambda)$ is the characteristic polynomial of A, $\chi(\lambda) = (\lambda - k)\chi_1(\lambda)$. By Cayley–Hamilton theorem, $\chi(A) = 0$ and hence we have $A\chi_1(A) = k\chi_1(A)$. Hence, every column vector of $\chi_1(A)$ is an eigenvector of A corresponding to the eigenvalue k. But by Theorem 11.5.1, the space of eigenvectors of A is generated by $\mathbf{1}$, G being connected. Hence, each column vector of $\chi_1(A)$ is a multiple of $\mathbf{1}$. But $\chi_1(A)$ is symmetric and hence $\chi_1(A)$ is a multiple of J, say, $\chi_1(A) = \alpha J$, $\alpha \neq 0$. Thus, J and hence $J - I - A$ are polynomials in A (remember: $A^0 = I$). Let $\lambda \neq k$ be any eigenvalue of A [so that $\chi_1(\lambda) = 0$], and Y an eigenvector of A corresponding to λ. Then

$$\begin{aligned} A^c Y &= (J - I - A)Y \\ &= \left(\frac{\chi_1(A)}{\alpha} - I - A\right)Y \\ &= \left(\frac{\chi_1(\lambda)}{\alpha} - 1 - \lambda\right)Y \text{ (see Note 11.5.4 below)} \\ &= (-1 - \lambda)Y. \end{aligned}$$

Thus, $A^c Y = (-1-\lambda)Y$, and therefore $-1-\lambda$ is an eigenvalue of A^c corresponding to the eigenvalue $\lambda(\neq k)$ of A. □

Note 11.5.4. We recall that if $f(\lambda)$ is a polynomial in λ, and $Sp(A) = \begin{pmatrix} \lambda_1 & \lambda_2 & \cdots & \lambda_s \\ m_1 & m_2 & \cdots & m_s \end{pmatrix}$, then $Sp(f(A)) = \begin{pmatrix} f(\lambda_1) & f(\lambda_2) & \cdots & f(\lambda_s) \\ m_1 & m_2 & \cdots & m_s \end{pmatrix}$.

11.5.2 Spectra of Line Graphs of Regular Graphs

We now establish Sachs' theorem, which determines the spectrum of the line graph of a regular graph G in terms of $Sp(G)$.

Let G be a labeled graph with vertex set $V(G) = \{v_1, \ldots, v_n\}$ and edge set $E(G) = \{e_1, \ldots, e_m\}$. With respect to these labelings, the incidence matrix $B = (b_{ij})$ of G, which describes the incidence structure of G, is defined as the m by n matrix $B = (b_{ij})$, where $b_{ij} = \begin{cases} 1 & \text{if } e_i \text{ is incident to } v_j, \\ 0 & \text{otherwise.} \end{cases}$

Lemma 11.5.5. *Let G be a graph of order n and size m with A and B as its adjacency and incidence matrices, respectively. Let A_L denote the adjacency matrix of the line graph of G. Then*

(i) $BB^{\mathrm{T}} = A_L + 2I_m$.
(ii) If G is k-regular, $B^{\mathrm{T}}B = A + kI_n$.

Proof. Let $A = (a_{ij})$ and $B = (b_{ij})$. We have

(i)

$$
\begin{aligned}
(BB^{\mathrm{T}})_{ij} &= \sum_{p=1}^{n} b_{ip} b_{jp} \\
&= \text{number of vertices } v_p \text{ that are incident to both } e_i \text{ and } e_j \\
&= \begin{cases} 1 & \text{if } e_i \text{ and } e_j \text{ are adjacent} \\ 0 & \text{if } i \neq j \text{ and } e_i \text{ and } e_j \text{ are nonadjacent} \\ 2 & \text{if } i = j. \end{cases}
\end{aligned}
$$

(ii) Proof of (ii) is similar. □

Theorem 11.5.6 (Sachs' theorem). *Let G be a k-regular graph of order n. Then $\chi(L(G); \lambda) = (\lambda + 2)^{m-n} \chi(G; \lambda + 2 - k)$, where $L(G)$ is the line graph (see Chap. 1) of G.*

Proof. Consider the two partitioned matrices U and V, each of order $n + m$ (where B stands for the incidence matrix of G):

$$U = \begin{bmatrix} \lambda I_n & -B^{\mathrm{T}} \\ 0 & I_m \end{bmatrix}, \; V = \begin{bmatrix} I_n & B^{\mathrm{T}} \\ B & \lambda I_m \end{bmatrix}.$$

We have

$$UV = \begin{bmatrix} \lambda I_n - B^{\mathrm{T}} B & 0 \\ B & \lambda I_m \end{bmatrix} \text{ and } VU = \begin{bmatrix} \lambda I_n & 0 \\ \lambda B & \lambda I_m - BB^{\mathrm{T}} \end{bmatrix}.$$

Now $\det(UV) = \det(VU)$ gives:

$$\lambda^m \det(\lambda I_n - B^{\mathrm{T}} B) = \lambda^n \det(\lambda I_m - BB^{\mathrm{T}}). \tag{11.1}$$

Replacement of λ by $\lambda + 2$ in (11.1) yields

$$(\lambda + 2)^{m-n} \det((\lambda + 2) I_n - B^{\mathrm{T}} B) = \det((\lambda + 2) I_m - BB^{\mathrm{T}}). \tag{11.2}$$

Hence, by Lemma 11.5.5,

$$
\begin{aligned}
\chi(L(G); \lambda) &= \det(\lambda I_m - A_L) \\
&= \det((\lambda + 2) I_m - (A_L + 2 I_m)) \\
&= \det((\lambda + 2) I_m - BB^{\mathrm{T}}) \\
&= (\lambda + 2)^{m-n} \det((\lambda + 2) I_n - B^{\mathrm{T}} B) \quad \text{(by (11.2))}
\end{aligned}
$$

$$= (\lambda + 2)^{m-n} \det((\lambda + 2)I_n - (A + kI_n)) \quad \text{(by Lemma 11.5.5)}$$
$$= (\lambda + 2)^{m-n} \det((\lambda + 2 - k)I_n - A)$$
$$= (\lambda + 2)^{m-n} \chi(G; \lambda + 2 - k).$$

□

Sachs' theorem implies the following: As $\chi(G;\lambda) = \prod_1^n (\lambda - \lambda_i)$, it follows that

$$\chi(L(G);\lambda) = (\lambda + 2)^{m-n} \prod_{i=1}^{n} (\lambda + 2 - k - \lambda_i)$$
$$= (\lambda + 2)^{m-n} \prod_{i=1}^{n} \Big(\lambda - (k - 2 + \lambda_i)\Big).$$

Hence if $Sp(G) = \begin{pmatrix} k & \lambda_2 & \dots & \lambda_s \\ 1 & m_2 & \dots & m_s \end{pmatrix}$, then

$$Sp(L(G)) = \begin{pmatrix} 2k-2 & k-2+\lambda_2 & \dots & k-2+\lambda_s & -2 \\ 1 & m_2 & \dots & m_s & m-n \end{pmatrix}.$$

We note that the spectrum of the Petersen graph can be obtained by using Theorems 11.5.3 and 11.5.6 (see Exercise 14.14). We use this result to prove a well-known result on the Petersen graph.

Theorem 11.5.7. *The complete graph K_{10} cannot be decomposed into (that is, expressed as an edge-disjoint union of) three copies of the Petersen graph.*

Proof (Schwenk and Lossers [169]). Assume the contrary. Suppose K_{10} is expressible as an edge-disjoint union of three copies, say, P_1, P_2, P_3, of the Petersen graph P (see Fig. 11.1). Then

$$A(K_{10}) = J - I = A(P_1) + A(P_2) + A(P_3), \tag{11.3}$$

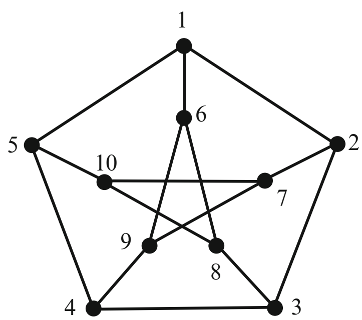


Fig. 11.1 Petersen graph P

where $A(H)$ stands for the adjacency matrix of the graph H, and J the all-1 matrix of order 10. (Note that each P_i is a spanning subgraph of K_{10}, that the number of edges of P_i, namely 15, is a divisor of the number of edges of K_{10}, namely, 45, and that the degree of any vertex v of P, namely, 3, is a divisor of the degree of v in K_{10}, namely 9.) It is easy to check that 1 is an eigenvalue of P. Further, as P is 3-regular, the all-1 column vector $\mathbf{1}$ is an eigenvector of P. Now $\mathbb{R}^{10}$ has an orthonormal basis of eigenvectors of $A(P)$ containing $\mathbf{1}$. Again, the null space of $(A(P)-1.I) = A(P)-I$ is of dimension 5 and is orthogonal to $\mathbf{1}$. (For P with the labeling of Fig. 11.1, one can check that for $A(P) - I$, the null space is spanned by the five vectors: $(1\ 0\ 0\ 0\ 0\ 1\ -1\ 0\ 0\ -1)^T$, $(0\ 1\ 0\ 0\ 0\ -1\ 1\ -1\ 0\ 0)^T$, $(0\ 0\ 1\ 0\ 0\ 0\ -1\ 1\ -1\ 0)^T$, $(0\ 0\ 0\ 1\ 0\ 0\ 0\ -1\ 1\ -1)^T$, $(0\ 0\ 0\ 0\ 1\ -1\ 0\ 0\ -1\ 1)^T$) The orthogonal complement of $\mathbf{1}$ in $\mathbb{R}^{10}$ is of dimension $10 - 1 = 9$. Hence, the null spaces of $A(P_1) - I$ and $A(P_2) - I$ must have a common eigenvector $\mathbf{x}$ orthogonal to $\mathbf{1}$. Multiplying the matrices on the two sides of (11.3) to $\mathbf{x}$, we get $(J - I)\mathbf{x} = A(P_1)\mathbf{x} + A(P_2)\mathbf{x} + A(P_3)\mathbf{x}$, that is (as $J\mathbf{x} = 0$), $-\mathbf{x} = \mathbf{x} + \mathbf{x} + A(P_3)\mathbf{x}$. Thus, $A(P_3)\mathbf{x} = -3\mathbf{x}$, and this means that -3 is an eigenvalue of the Petersen graph, a contradiction (see Exercise 14.14). □

Various proofs of Theorem 11.5.7 are available in literature. For a second proof, see [32].

11.6 Spectrum of the Complete Bipartite Graph $K_{p,q}$

We now determine the spectrum of the complete bipartite graph $K_{p,q}$.

Theorem 11.6.1. $Sp(K_{p,q}) = \begin{pmatrix} 0 & \sqrt{pq} & -\sqrt{pq} \\ p+q-2 & 1 & 1 \end{pmatrix}$.

Proof. Let $V(K_{p,q})$ have the bipartition (X, Y) with $|X| = p$ and $|Y| = q$. Then the adjacency matrix of $K_{p,q}$ is of the form

$$A = \begin{pmatrix} 0 & J_{p,q} \\ J_{q,p} & 0 \end{pmatrix},$$

where $J_{r,s}$ stands for the all-1 matrix of size r by s. Clearly, rank(A) = 2, as the maximum number of independent rows of A is 2. Hence, zero is an eigenvalue of A repeated $p + q - 2$ times (as the null space of A is of dimension $p + q - 2$). Thus, the characteristic polynomial of A is of the form $\lambda^{p+q-2}(\lambda^2 + c_2)$.

[Recall that by Lemma 11.4.1, the coefficient of λ^{p+q-1} in $\chi(G;\lambda)$ is zero.] Further, again by the same lemma, $-c_2 =$ the number of edges of $K_{p,q} = pq$. This proves the result. □

11.7 The Determinant of the Adjacency Matrix of a Graph

We now present the elegant formula given by Harary for the determinant of the adjacency matrix of a graph in terms of certain of its subgraphs.

Definition 11.7.1. A *linear subgraph* of a graph G is a subgraph of G whose components are single edges or cycles.

Theorem 11.7.2 (Harary [92]). *Let A be the adjacency matrix of a simple graph G. Then*

$$\det A = \sum_{H} (-1)^{e(H)} 2^{c(H)},$$

where the summation is over all the spanning linear subgraphs H of G, and $e(H)$ and $c(H)$ denote, respectively, the number of even components and the number of cycles in H.

Proof. Let G be of order n with $V = \{v_1, \ldots, v_n\}$, and $A = (a_{ij})$. A typical term in the expansion of $\det A$ is

$$sgn(\pi) a_{1\pi(1)} a_{2\pi(2)} \ldots a_{n\pi(n)},$$

where π is a permutation on $\{1, 2, \ldots, n\}$ and $sgn(\pi) = 1$ or -1 according to whether π is an even or odd permutation. This term is zero if and only if for some i, $1 \leq i \leq n$, $a_{i\pi(i)} = 0$, that is, if and only if $\pi(i) = i$ or $\pi(i) = j (\neq i)$ and $v_i v_j \notin E(G)$. Hence, this term is nonzero if and only if the permutation π is a product of disjoint cycles of length *at least* 2, and in this case, the value of the term is $sgn(\pi).1.1 \ldots 1 = sgn(\pi)$. Each cycle (ij) of length 2 in π corresponds to the single edge $v_i v_j$ of G, while each cycle $(ij \ldots p)$ of length $r > 2$ in π corresponds to a cycle of length r of G. Thus, each nonvanishing term in the expansion of $\det A$ gives rise to a linear subgraph H of G and conversely. Now for any cycle C of S_n, $sgn(C) = 1$ or -1 according to whether C is an odd or even cycle. Hence, $sgn(\pi) = (-1)^{e(H)}$, where $e(H)$ is the number of even components of H (that is, components that are either single edges or even cycles of the graph H). Moreover, any cycle of H has two different orientations. Hence, each of the undirected cycles of H of length ≥ 3 yields two distinct even cycles in S_n. [For example, the 4-cycle $(v_{i_1} v_{i_2} v_{i_3} v_{i_4})$ gives rise to two cycles $(v_{i_1} v_{i_2} v_{i_3} v_{i_4})$ and $(v_{i_4} v_{i_3} v_{i_2} v_{i_1})$ in H.] This proves the result. □

Corollary 11.7.3 (Sachs [167]). *Let $\chi(G; x) = x^n + a_1 x^{n-1} + \cdots + a_n$ be the characteristic polynomial of G. Then*

$$a_i = \sum_{H} (-1)^{\omega(H)} 2^{c(H)},$$

where the summation is over all linear subgraphs H of order i of G, and $\omega(H)$ and $c(H)$ denote, respectively, the number of components and the number of cycle components of H.

Proof. Recall that $a_i = (-1)^i \sum_H \det A$, where H runs through all the induced subgraphs of order i of G. But by Theorem 11.7.2,

$$\det H = \sum_{H_i} (-1)^{e(H_i)} 2^{c(H_i)},$$

where H_i is a spanning linear subgraph of H and $e(H_i)$ stands for the number of even components of H_i, while $c(H_i)$ stands for the number of cycles in H_i. The corollary follows from the fact that i and the number of odd components of H_i have the same parity. □

11.8 Spectra of Product Graphs

We have already defined in Chap. 1 the graph products: Cartesian product, direct product, and strong product. In this section we determine the spectra of these graphs in terms of the spectra of their factor graphs. Our approach is based on Cvetković [46] as described in [47]. Recall that all these three products are associative.

Let $\mathscr{B}$ be a set of binary n-tuples $(\beta_1, \beta_2, \ldots, \beta_n)$ not containing $(0, 0, \ldots, 0)$.

Definition 11.8.1. Given a sequence of graphs $G_1, G_2, \ldots, G_n$, the *NEPS* (*Non-complete Extended P-Sum*) of $G_1, G_2, \ldots, G_n$, with respect to $\mathscr{B}$ is the graph G with $V(G) = V(G_1) \times V(G_2) \times \ldots \times V(G_n)$, and in which two vertices $(x_1, x_2, \ldots, x_n)$ and $(y_1, y_2, \ldots, y_n)$ are adjacent if and only if there exists an n-tuple $(\beta_1, \beta_2, \ldots, \beta_n) \in \mathscr{B}$ with the property that if $\beta_i = 1$, then $x_i y_i \in E(G_i)$ and if $\beta_i = 0$, then $x_i = y_i$.

Example 11.8.2. (i) $n = 2$ and $\mathscr{B} = \{(1, 1)\}$. Here the graphs are G_1 and G_2. The vertices (x_1, x_2) and (y_1, y_2) are adjacent in the NEPS of G_1 and G_2 with respect to $\mathscr{B}$ if and only if $x_1 y_1 \in E(G_1)$ and $x_2 y_2 \in E(G_2)$. Hence, $G = G_1 \times G_2$, the *direct product* of G_1 and G_2.

(ii) $n = 2$ and $\mathscr{B} = \{(0, 1), (1, 0)\}$. Here G is the Cartesian product $G_1 \Box G_2$.

(iii) $n = 2$ and $\mathscr{B} = \{(0, 1), (1, 0), (1, 1)\}$. Here $G = (G_1 \Box G_2) \cup (G_1 \times G_2) = G_1 \boxtimes G_2$, the strong product of G_1 and G_2.

Now, given the adjacency matrices of $G_1, \ldots G_n$, the adjacency matrix of the NEPS graph G with respect to the basis $\mathscr{B}$ is expressible in terms of the Kronecker product of matrices, which we now define:

Definition 11.8.3. Let $A = (a_{ij})$ be an m by n matrix and $B = (b_{ij})$ be a p by q matrix. Then $A \otimes B$, the *Kronecker product of A with B,* is the mp by nq matrix obtained by replacing each entry a_{ij} of A by the double array $a_{ij} B$ (where $a_{ij} B$ is the matrix obtained by multiplying each entry of B by a_{ij}).

It is well known and easy to check that

$$(A \otimes B)(C \otimes D) = (AC \otimes BD), \tag{11.4}$$

whenever the matrix products AC and BD are defined. Clearly, this can be extended to any finite product whenever the products are defined.

Remark 11.8.4. Let us look more closely at the product $A_1 \otimes A_2$, where A_1 and A_2 are the adjacency matrices of the graphs G_1 and G_2 of orders n and t, respectively. To fix any particular entry of $A_1 \otimes A_2$, let us first label $V(G_1) = V_1$ and $V(G_2) = V_2$ as $V_1 = \{u_1, \ldots, u_n\}$, and $V_2 = \{v_1, \ldots, v_t\}$. Then to fix the entry in $A_1 \otimes A_2$ corresponding to $\big((u_i, u_j),\ (v_p, v_q)\big)$, we look at the double array $(A_1)_{(u_i u_j)} A_2$ in $A_1 \otimes A_2$, where $(A_1)_{(u_i u_j)} := \alpha$ stands for the (i, j)th entry of A_1. Then the required entry is just $\alpha\{(p, q)$th entry of $A_2\}$. Hence, it is $\mathbf{1}$ if and only if $(A_1)_{(u_i u_j)} = 1 = (A_2)_{(v_p v_q)}$, that is, if and only if $u_i u_j \in E(G_1)$ and $v_p v_q \in E(G_2)$, and 0 otherwise. In other words, $A_1 \otimes A_2$ is the adjacency matrix of $G_1 \times G_2$. By associativity, $A(G_1) \otimes \ldots \otimes A(G_r)$ is the adjacency matrix of the graph product $G_1 \times \ldots \times G_r$.

Our next theorem determines the adjacency matrix of the NEPS G in terms of the adjacency matrices of G_i, $1 \le i \le n$ for all three products mentioned above.

Theorem 11.8.5 (Cvetković [46]). *Let G be the NEPS of the graphs $G_1, \ldots, G_n$ with respect to the basis $\mathscr{B}$. Let A_i be the adjacency matrix of G_i, $1 \le i \le n$. Then the adjacency matrix A of G is given by*

$$A = \sum_{\beta = (\beta_1, \ldots, \beta_n) \in \mathscr{B}} A_1^{\beta_1} \otimes \ldots \otimes A_n^{\beta_n}.$$

Proof. Label the vertex set of each of the graphs G_i, $1 \le i \le n$, and order the vertices of G lexicographically. Form the adjacency matrix A of G with respect to this ordering. Then (by the description of Kronecker product of matrices given in Remark 11.8.4) we have $(A)_{(x_1,\ldots,x_n)(y_1,\ldots,y_n)} = \sum_{\beta \in \mathscr{B}} (A_1^{\beta_1})_{(x_1,y_1)} \cdots (A_n^{\beta_n})_{(x_n,y_n)}$, where $(M)_{(x,y)}$ stands for the entry in M corresponding to the vertices x and y. But by lexicographic ordering, $(M)_{(x_1,\ldots,x_n)(y_1,\ldots,y_n)} = 1$ if and only if there exists a $\beta = (\beta_1, \ldots, \beta_n) \in \mathscr{B}$ with $(A_i^{\beta_i})_{(x_i,y_i)} = 1$ for each $i = 1, \ldots, n$. This of course means that $x_i y_i \in E(G_i)$ if $\beta_i = 1$ and $x_i = y_i$ if $\beta_i = 0$ (the latter condition corresponds to $A_i^{\beta_i} = I$). □

We now determine the spectrum of the NEPS graph G with respect to the basis $\mathscr{B}$ in terms of the spectra of the factor graphs G_i.

Theorem 11.8.6 (Cvetković [46]). *Let G be the NEPS of the graphs $G_1, \ldots, G_n$ with respect to the basis $\mathscr{B}$. Let k_i be the order of G_i and A_i, the adjacency matrix of G_i. Let $\{\lambda_{i1}, \ldots, \lambda_{ik_i}\}$ be the spectrum of G_i, $1 \le i \le n$. Then*

$$Sp(G) = \{\Lambda_{i_1 i_2 \ldots i_n} : 1 \le i_j \le k_j \text{ and } 1 \le j \le n\},$$

where $\Lambda_{i_1 i_2 \ldots i_n} = \sum_{\beta = (\beta_1, \ldots, \beta_n) \in \mathscr{B}} \lambda_{1 i_1}^{\beta_1} \ldots, \lambda_{n i_n}^{\beta_n}$, $1 \le i_j \le k_j$ and $1 \le j \le n$.

Proof. There exist vectors x_{ij} with $A_i x_{ij} = \lambda_{ij} x_{ij}$, $1 \leq i \leq n$; $1 \leq j \leq k_j$. Now consider the vector $\mathrm{x} = x_{1i_1} \otimes \ldots \otimes x_{ni_n}$. Let A be the adjacency matrix of G. Then from Theorem 11.8.5 and (11.4) (rather its extension),

$$\begin{aligned} A\mathrm{x} &= \left(\sum_{\beta \in \mathscr{B}} A_1^{\beta_1} \otimes \ldots \otimes A_n^{\beta_n} \right) (x_{1i_1} \otimes \ldots \otimes x_{ni_n}) \\ &= \sum_{\beta \in \mathscr{B}} (A_1^{\beta_1} x_{1i_1} \otimes \ldots \otimes A_n^{\beta_n} x_{ni_n}) \\ &= \sum_{\beta \in \mathscr{B}} (\lambda_{1i_1}^{\beta_1} x_{1i_1} \otimes \ldots \otimes \lambda_{ni_n}^{\beta_n} x_{ni_n}) \\ &= \left(\sum_{\beta \in \mathscr{B}} \lambda_{1i_1}^{\beta_1} \ldots \lambda_{ni_n}^{\beta_n} \right) \mathrm{x} \\ &= \Lambda_{i_1 i_2 \ldots i_n} \mathrm{x}. \end{aligned}$$

Thus, $\Lambda_{i_1 i_2 \ldots i_n}$ is an eigenvalue of G. This yields $k_1 k_2 \ldots k_n$ eigenvalues of G and hence all the eigenvalues of G. □

Corollary 11.8.7. *Let $Sp(G_1) = \{\lambda_1, \ldots, \lambda_n\}$ and $Sp(G_2) = \{\mu_1, \ldots, \mu_t\}$ and let A_1 and A_2 be the adjacency matrices of G_1 and G_2, respectively. Then*

(i) $A(G_1 \times G_2) = A_1 \otimes A_2$; *and* $Sp(G_1 \times G_2) = \{\lambda_i \mu_j : 1 \leq i \leq n, 1 \leq j \leq t\}$.
(ii) $A(G_1 \Box G_2) = (I_n \otimes A_2) + (A_1 \otimes I_t)$; *and* $Sp(G_1 \Box G_2) = \{\lambda_i + \mu_j : 1 \leq i \leq n, 1 \leq j \leq t\}$.
(iii) $A(G_1 \boxtimes G_2) = (A_1 \otimes A_2) + (I_n \otimes A_2) + (A_1 \otimes I_t)$; *and* $Sp(G_1 \boxtimes G_2) = \{\lambda_i \mu_j + \lambda_i + \mu_j : 1 \leq i \leq n, 1 \leq j \leq t\}$.

□

11.9 Cayley Graphs

11.9.1 Introduction

Cayley graphs are a special type of regular graphs constructed out of groups.

Let Γ be a finite group and $S \subset \Gamma$ be such that

(i) $e \notin S$ (e is the identity of Γ),
(ii) If $a \in S$, then $a^{-1} \in S$, and
(iii) S generates Γ.

Construct a graph G with $V(G) = \Gamma$ and in which $ab \in E(G)$ if and only if $b = as$ for some $s \in S$. Since $as = as'$ in Γ implies that $s = s'$, it follows that each vertex a of G is of degree $|S|$; that is, G is a $|S|$-regular graph. Moreover, if a and b are any two vertices of G, there exists c in Γ such that $ac = b$. But as S generates Γ, $c = s_1 s_2 \ldots s_p$, where $s_i \in S$, $1 \leq i \leq p$. Hence, $b = as_1 s_2 \ldots s_p$, which implies that b is reachable from a in G by means of the path $a(as_1)(as_1 s_2) \ldots (as_1 s_2 \ldots s_p = b)$. Thus, G is a connected simple graph. [Condition (i) implies that G has no loops.] G is known as the *Cayley graph* $\mathrm{Cay}(\Gamma; S)$ of the group Γ defined by the set S.

We now consider a special family of Cayley graphs. Take $\Gamma = (\mathbb{Z}_n, +)$, the additive group of integers modulo n. If $S = \{s_1, s_2, \ldots, s_p\}$, then $0 \notin S$ and $s_i \in S$ if and only if $n - s_i \in S$. The vertices adjacent to 0 are $s_1, s_2, \ldots, s_p$, while those adjacent to i are $(s_1 + i)(\mathrm{mod}\ n), (s_2 + i)(\mathrm{mod}\ n), \ldots, (s_p + i)(\mathrm{mod}\ n)$. Consequently, the adjacency matrix of $\mathrm{Cay}(\mathbb{Z}_n; S)$ is a circulant and, by Lemma 11.2.3, its eigenvalues are

$$\{\omega^{s_1} + \omega^{s_2} + \cdots + \omega^{s_p} \ : \ \omega = \text{an } n\text{th root of unity}\}.$$

11.9.2 Unitary Cayley Graphs

We now take $S(\subset \mathbb{Z}_n)$ to be the set U_n of numbers less than n and prime to n. Note that $(a, n) = 1$ if and only if $(n - a, n) = 1$. The corresponding Cayley graph $\mathrm{Cay}(\mathbb{Z}_n; U_n)$ is denoted by X_n and called the *unitary Cayley graph* mod n (Note that U_n is the set of multiplicative units in $\mathbb{Z}_n$.) Now suppose that $(n_1, n_2) = 1$. What is the Cayley graph $X_{n_1 n_2}$? Given $x \in \mathbb{Z}_{n_1 n_2}$, there exist unique $c \in \mathbb{Z}_{n_1}$ and $d \in \mathbb{Z}_{n_2}$ such that

$$x \equiv c(\mathrm{mod}\ n_1) \quad \text{and} \quad x \equiv d(\mathrm{mod}\ n_2). \tag{11.5}$$

Conversely, given $c \in \mathbb{Z}_{n_1}$ and $d \in \mathbb{Z}_{n_2}$, by the Chinese Remainder Theorem [5], there exists a unique $x \in \mathbb{Z}_{n_1 n_2}$ satisfying (11.5). Define $f : \mathbb{Z}_{n_1 n_2} \to \mathbb{Z}_{n_1} \times \mathbb{Z}_{n_2}$ (the direct product of the groups Z_{n_1} and Z_{n_2}) by setting $f(x) = (c, d)$. Then f is an additive group isomorphism with $f(U_{n_1 n_2}) = U_{n_1} \times U_{n_2}$.

Two vertices a and b are adjacent in $\mathbb{Z}_{n_1 n_2}$ if and only if $a - b \in U_{n_1 n_2}$. Let

$$a \equiv a_1(\mathrm{mod}\ n_1), \qquad b \equiv b_1(\mathrm{mod}\ n_1)$$
$$a \equiv a_2(\mathrm{mod}\ n_2) \quad \text{and} \quad b \equiv b_2(\mathrm{mod}\ n_2).$$

Then $(a - b, n_1 n_2) = 1$ if and only if $(a - b, n_1) = 1 = (a - b, n_2)$; equivalently, $(a_1 - b_1, n_1) = 1 = (a_2 - b_2, n_2)$ or, in other words, $a_1 b_1 \in E(X_{n_1})$ and $a_2 b_2 \in E(X_{n_2})$. Thus, we have the following result.

Theorem 11.9.1. *If $(n_1, n_2) = 1$, the unitary Cayley graph $X_{n_1 n_2}$ is isomorphic to $X_{n_1} \times X_{n_2}$ (where $\times$ on the right stands for direct product of graphs).*

11.9.3 Spectrum of the Cayley Graph X_n

The adjacency matrix of X_n, as noted before, is a circulant, and hence the spectrum $(\lambda_1, \lambda_2, \ldots, \lambda_n)$ of X_n (see the proof of Lemma 11.2.3) is given by

$$\lambda_r = \sum_{\substack{1 \le j \le n, \\ (j,n)=1}} \omega^{rj}, \quad \text{where } \omega = e^{\frac{2\pi i}{n}}. \tag{11.6}$$

The sum in (11.6) is the well-known Ramanujan sum $c(r,n)$ [123]. It is known that

$$c(r,n) = \mu(t_r)\frac{\phi(n)}{\phi(t_r)}, \text{ where } t_r = \frac{n}{(r,n)}, \ 0 \le r \le n-1. \tag{11.7}$$

In relation (11.7), μ stands for the Möebius function. Further, as t_r divides n, $\phi(t_r)$ divides $\phi(n)$, and therefore $c(r,n)$ is an integer for each r. These remarks yield the following theorem.

Theorem 11.9.2. *The eigenvalues of the unitary Cayley graph* $X_n = \text{Cay}(\mathbb{Z}_n, U_n)$ *are all the integers* $c(r,n)$, $0 \le r \le n-1$.

For more spectral properties of Cayley graphs, the reader may consult Klotz and Sander [123].

11.10 Strongly Regular Graphs

Strongly regular graphs form an important class of regular graphs.

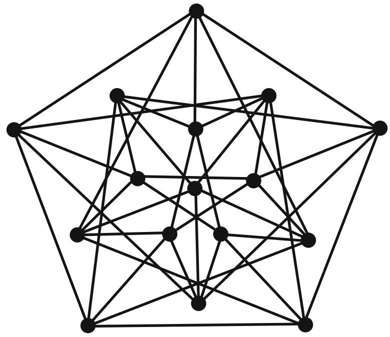
Definition 11.10.1. A *strongly regular graph* with parameters (n,k,λ,μ) (for short: $srg(n,k,\lambda,\mu)$) is a k-regular connected graph G of order n with the following properties:

(i) Any two adjacent vertices of G have exactly λ common neighbors in G.
(ii) Any two nonadjacent vertices of G have exactly μ common neighbors in G.

Example 11.10.2. (i) The cycle C_5 is an $srg(5,2,0,1)$.
(ii) The Petersen graph P is an $srg(10,3,0,1)$.
(iii) The cycle C_6 is a regular graph that is not strongly regular.
(iv) The Clebesch graph is an $srg(16,5,0,2)$ (see Fig. 11.2).
(v) Let $q \equiv 1 (\text{mod } 4)$ be an odd prime power. The *Paley graph* $P(q)$ of order q is the graph with vertex set $GF(q)$, the Galois field of order q, with two vertices adjacent in $P(q)$ if and only if their difference is a nonzero square in $GF(q)$. $P(q)$ is an $srg(q, \frac{1}{2}(q-1), \frac{1}{4}(q-5), \frac{1}{4}(q-1))$.

Our next theorem gives a necessary condition for the existence of a strongly regular graph with parameters (n,k,λ,μ).

Fig. 11.2 Clebsch Graph



Theorem 11.10.3. *If G is a strongly regular graph with parameters (n, k, λ, μ), then*

$$k(k - \lambda - 1) = \mu(n - k - 1).$$

Proof. We prove this theorem by counting the number of induced paths on three vertices in G having the same vertex v of G as an end vertex in two different ways. There are k neighbors w of v in G. For each such w, there are λ vertices that are common neighbors of v and w. Each of the remaining $k - 1 - \lambda$ neighbors of w induces a P_3 with v as an end vertex. As this is true for each neighbor w of v in G, there are $k(k - \lambda - 1)$ paths of length 2 with v as an end vertex.

We now compute this number in a different way. There are $n-1-k$ vertices x of G that are nonadjacent to v. Each such pair v, x is commonly adjacent to μ vertices of G. Each one of these μ vertices gives rise to an induced P_3 in G with v as an end vertex. This number is $\mu(n - k - 1)$. □

Suppose now $\lambda = k - 1$. As G is k-regular, $ab \in E(G)$, implies that every vertex c adjacent to a is adjacent to b, and every vertex d adjacent to b is adjacent to a. Now consider the adjacent pair b, c. Then c must be adjacent to d and so on. Thus, each component of G must be a clique (complete subgraph) of size k.

A similar reasoning applies when $\mu = 0$. Further, if $k = n - 1$, G is K_n, the clique on n vertices. We treat these cases (that is, the cases when $\lambda = k - 1; \mu = 0; k = n - 1$) as degenerate cases.

Theorem 11.10.4. *If G is an $srg(n, k, \lambda, \mu)$, then its complement G^c of G is an $srg(n, n-1-k, n-2-2k+\mu, n-2k+\lambda)$.*

Proof. Trivially, G^c is $n - 1 - k$ regular. Suppose now $uv \in E(G^c)$. Then $uv \notin E(G)$. There are k vertices adjacent to u in G and k vertices adjacent to v in G. Out of these $2k$ vertices, μ are common vertices adjacent to both u and v in G^c. Hence, there are $(n - 2) - (2k - \mu) = n - 2 - 2k + \mu$ vertices commonly adjacent to u and v in G^c. By a similar argument, if $uv \notin E(G^c)$, u and v are commonly adjacent to $n - 2k + \lambda$ vertices in G^c. Thus, G^c is an $srg(n, n - 1 - k, n - 2 - 2k + \mu, n - 2k + \lambda)$. □

We now present another necessary condition for a graph to be strongly regular.

Theorem 11.10.5. *If G is an $srg(n, k, \lambda, \mu)$, with $\mu > 0$, then the two numbers*

$$\frac{1}{2}\left(n - 1 \pm \frac{(n-1)(\mu-\lambda) - 2k}{\sqrt{(\mu-\lambda)^2 + 4(k-\mu)}}\right)$$

are both nonnegative integers.

Proof. We prove the theorem by showing that the two numbers are (algebraic) multiplicities of eigenvalues of G. If A is the adjacency matrix of G, $J - I - A$ (where J is the all-1 matrix of order n) is the adjacency matrix of G^c. What is the (i, j)th entry of A^2? If $i = j$, the number of v_i-v_j walks of length 2 is k since they are all of the form $v_i v_p v_i$, and there are k adjacent vertices v_p to v_i in G. Hence, each diagonal entry of A^2 is k.

Now let $i \neq j$. Then $v_i v_j \in E(G)$ if and only if $v_i v_j \notin E(G^c)$. Hence if $i \neq j$, the (i, j)th entry is 1 or 0 in A if and only if the (i, j)th entry is 0 or 1, respectively, in $J - I - A$. Now there are exactly λ vertices commonly adjacent to v_i and v_j in G, and hence there are λ paths of length 2 in G. Hence, the 1's in A will be replaced by λ in A^2, and this is given by the matrix λA. Finally, let $i \neq j$ and $v_i v_j \notin E(G)$. The number of v_i-v_j walks of length 2 in G is μ. The (i, j)th entry 0 in A should now be replaced by μ. This can be done by replacing the (i, j)th entry 1 in $(J - I - A)$ by μ. Thus,

$$A^2 = kI + \lambda A + \mu(J - I - A). \tag{11.8}$$

Hence, if $\mathbf{1}$ is the column vector $(1, 1, \ldots, 1)^{\mathrm{T}}$ of length n,

$$A^2\mathbf{1} = (kI + \lambda A + \mu(J - I - A))\mathbf{1},$$

and this gives (as $A\mathbf{1} = k\mathbf{1}$)

$$k^2\mathbf{1} = k\mathbf{1} + \lambda k\mathbf{1} + \mu(n - 1 - k)\mathbf{1}. \tag{11.9}$$

Note that (11.9) yields another proof for Theorem 11.10.3.

Now as G is connected, $\mathbf{1}$ is a unique eigenvector corresponding to the eigenvalue k of G. Let $\mathbf{x}$ be any eigenvector corresponding to an eigenvalue $\theta \neq k$ of G so that $A\mathbf{x} = \theta\mathbf{x}$. Then $\mathbf{x}$ is orthogonal to $\mathbf{1}$. Taking the product of both sides of (11.8) with $\mathbf{x}$, we get (as $J\mathbf{x} = 0$)

$$\theta^2\mathbf{x} = A^2\mathbf{x} = k\mathbf{x} + \lambda\theta\mathbf{x} + \mu(-\mathbf{x} - \theta\mathbf{x}),$$

and therefore (as $\mathbf{x}$ is a nonzero vector),

$$\theta^2 - (\lambda - \mu)\theta - (k - \mu) = 0. \tag{11.10}$$

This quadratic equation has two real roots (being eigenvalues of G), say, r and s, which are given by

$$\frac{1}{2}\Big[(\lambda - \mu) \pm \sqrt{(\lambda-\mu)^2 + 4(k-\mu)}\Big]. \tag{11.11}$$

Denote the multiplicities of r and s by a and b. Now

$$k + ra + sb = 0 \text{ (sum of the eigenvalues)},$$
$$\text{and } 1 + a + b = n \text{ (total number of eigenvalues)}.$$

Solution of these equations gives

$$a = -\frac{k + s(n-1)}{r-s},$$
$$b = \frac{k + r(n-1)}{r-s}. \tag{11.12}$$

Substitution of the values of r and s as given in (11.11) into (11.12) yields the two numbers given in the statement of Theorem 11.10.5. □

11.11 Ramanujan Graphs

Ramanujan graphs constitute yet another family of regular graphs. In recent times, a great deal of interest has been shown in Ramanujan graphs by researchers in diverse fields—graph theory, number theory, and communication theory.

Definition 11.11.1. A *Ramanujan graph* is a k-regular connected graph G, $k \geq 2$, such that if λ is any eigenvalue of G with $|\lambda| \neq k$, then $\lambda \leq 2\sqrt{k-1}$.

Example 11.11.2. The following graphs are Ramanujan graphs.

1. The complete graphs K_n, $n \geq 3$.
2. Cycles C_n.
3. $K_{n,n}$. Here $k = n$, and $Sp(K_{n,n}) = \begin{pmatrix} n & 0 & -n \\ 1 & 2n-2 & 1 \end{pmatrix}$.
4. The Petersen graph.

The *Möebius ladder* M_h is the cubic graph obtained by joining the opposite vertices of the cycle C_{2h}. By Exercise 14.6, we have

$$\lambda_j = 2\cos\frac{\pi j}{h} + (-1)^j, \quad 0 \leq j \leq 2h-1.$$

Take $h = 2p$ and $j = 4p-2$. Then $\lambda_{4p-2} = 2\cos\frac{\pi(4p-2)}{2p} + 1 = 2\cos\frac{\pi}{p} + 1 > 2\sqrt{k-1}$ (when p becomes large) $= 2\sqrt{2}$ (as k $= 3$). Hence, not every regular graph is a Ramanujan graph.

11.11.1 Why Are Ramanujan Graphs Important?

Let G be a k-regular Ramanujan graph of order n, and A its adjacency matrix. As A is symmetric, $\mathbb{R}^n$ has an orthonormal basis $\{u_1, \ldots, u_n\}$ of eigenvectors of A. Since $A\mathbf{1} = k\mathbf{1}$, we can take $u_1 = (\frac{1}{\sqrt{n}}, \ldots, \frac{1}{\sqrt{n}})^{\mathrm{T}}$. Let $Sp(G) = \{\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n\}$, where $\lambda_1 = k$ and $Au_i = \lambda_i u_i$, $1 \leq i \leq n$. We can write $A = \sum_{i=1}^{n} \lambda_i u_i u_i^{\mathrm{T}}$. (This is seen from the fact that the matrices on the two sides when postmultiplied by u_j, $1 \leq j \leq n$ both yield $\lambda_j u_j$.) More generally, as λ_i^p, $1 \leq i \leq n$ are the eigenvalues of A^p, we have

$$A^p = \sum_{i=1}^{n} \lambda_i^p u_i u_i^{\mathrm{T}}. \tag{11.13}$$

Let $u_i = ((u_i)_1, (u_i)_2, \ldots, (u_i)_r, \ldots, (u_i)_n)$. Then the (r, s)th entry of $A^p = \sum_{i=1}^{n} \lambda_i^p (u_i)_r (u_i^{\mathrm{T}})_s = \sum_{i=1}^{n} \lambda_i^p (u_i)_r (u_i)_s := X_{rs}$. As A is a binary matrix, $X_{r,s}$ is a nonnegative integer. Moreover, as G is k-regular and connected, $\lambda_1 = k$. Set $\lambda(G) := \max_{|\lambda_i| \neq k} |\lambda_i|$. Then,

$$\begin{aligned}
X_{rs} &= \sum_{i=1}^{n} \lambda_i^p (u_i)_r (u_i)_s \\
&= \Big|\sum_{i=1}^{n} \lambda_i^p (u_i)_r (u_i)_s\Big| \\
&\geq k^p (u_1)_r (u_1)_s - \Big|\sum_{i=2}^{n} \lambda_i^p (u_i)_r (u_i)_s\Big| \\
&= k^p \frac{1}{\sqrt{n}} \frac{1}{\sqrt{n}} - |\Sigma_0|, \text{ where } \Sigma_0 = \sum_{i=2}^{n} \lambda_i^p (u_i)_r (u_i)_s. \qquad (11.14)
\end{aligned}$$

Assume that G is not bipartite, so that $\lambda_n \neq -k$ (see Exercise 14.22). Hence, the eigenvalues $\lambda_2, \ldots, \lambda_n$ all satisfy $|\lambda_i| \leq \lambda(G)$, and therefore

$$\begin{aligned}
|\Sigma_0| &\leq \lambda(G)^p \sum_{i=2}^{n} |(u_i)_r||(u_i)_s| \\
&\leq \lambda(G)^p \Big(\sum_{i=2}^{n} |(u_i)_r^2|\Big)^{1/2} \Big(\sum_{i=2}^{n} |(u_i)_s^2|\Big)^{1/2} \quad \text{(by Cauchy–Schwarz inequality)} \\
&= \lambda(G)^p \Big[1 - (u_1)_r^2\Big]^{1/2} \Big[1 - (u_1)_s^2\Big]^{1/2} \text{ (as the } u_i\text{'s are unit vectors)}
\end{aligned}$$

$$= \lambda(G)^p\left[1-\frac{1}{n}\right]^{1/2}\left[1-\frac{1}{n}\right]^{1/2}$$
$$= \lambda(G)^p\left[1-\frac{1}{n}\right].$$

Hence, the (r, s)th entry of A^p is positive if $\frac{k^p}{n} > \lambda(G)^p(1-\frac{1}{n})$, that is, if $\frac{k^p}{\lambda(G)^p} > n-1$.

This gives, on taking logarithms, that if

$$p > \frac{\log(n-1)}{\log\big(k/\lambda(G)\big)},$$

then every entry of A^p is positive. Now the diameter of G is the least positive integer p for which A^p is positive (see Exercise 14.3). Hence, the diameter D of G satisfies the inequality

$$D \leq \frac{\log(n-1)}{\log(k/\lambda(G))} + 1.$$

Thus, we have proved the following theorem.

Theorem 11.11.3 (Chung [37]). *Let G be a k-regular connected nonbipartite graph with n vertices and diameter D. Then*

$$D \leq \frac{\log(n-1)}{\log\big(k/\lambda(G)\big)} + 1. \tag{11.15}$$

Now assume that G is bipartite and k-regular. Then $\lambda_1 = k$ and $\lambda_n = -k$ so that $|\lambda_1| = k = |\lambda_n|$. Working as above, one gets the following inequality in this case:

$$D \leq \frac{\log(n-2)/2}{\log\big(k/\lambda(G)\big)} + 2. \tag{11.16}$$

The last two inequalities show that to minimize D, one has to minimize $\lambda(G) = \max_{|\lambda_i| \neq k} |\lambda_i|$. Such graphs are useful in communication theory—the smaller the diameter, better the communication. In the case of Ramanujan graphs, we demand that $\lambda(G) \leq 2\sqrt{k-1}$. Hence, Ramanujan graphs with sufficiently small values for $\lambda(G)$ could be used in cost-efficient communication networks.

We mention that in constructing k-regular Ramanujan graphs G for a fixed $k \geq 2$, it is not possible to bring down the upper bound $2\sqrt{k-1}$ for $\lambda(G)$ since as per a result of Serre [132], for $\epsilon > 0$, there exists a positive constant $c = c(k, \epsilon)$, which depends only on k and ϵ such that the adjacency matrix of every k-regular graph on n vertices has at least cn eigenvalues larger than $(2-\epsilon)\sqrt{k-1}$ (see also [137]). Again, not every unitary Cayley graph is a Ramanujan graph. Unitary Cayley graphs that are Ramanujan graphs have been completely characterized by Droll [58].

We conclude this section with a remark that explains the name "Ramanujan graph" (see also [162]). The question that one may ask is the following: Does there exist a sequence $\{G_i\}$ of graphs with an increasing number of vertices, satisfying the bound $\lambda(G_i) \leq 2\sqrt{k-1}$? That is, can we give an explicit construction for such a sequence of Ramanujan graphs? The only case known for which such sequences have been constructed is when $k-1$ equals a prime power. In all these cases, the proof that the eigenvalues satisfy the required bound is by means of the Ramanujan's conjecture in the theory of modular forms, proved by Deligne [48] in 1974 in the case when $k-1$ is a prime, and by the work of Drinfeld [57] in the case when $k-1$ is a prime power. This explains how Ramanujan's name has entered into the definition of these graphs.

We have only touched upon the periphery of Ramanujan graphs. A deeper study of Ramanujan graphs requires expertise in number theory. Interested readers can refer to the two survey articles by Ram Murty ([162, 163]) and the relevant references contained therein.

11.12 The Energy of a Graph

11.12.1 Introduction

In this section, we discuss another application of eigenvalues of graphs. "The energy of a graph" is a concept borrowed from chemistry. Every chemical molecule can be represented by means of its corresponding *molecular graph*: Each vertex of the graph corresponds to an atom of the molecule, and two vertices of the graph are adjacent if and only if there is a bond between the corresponding molecules (the number of bonds being immaterial). The π-electron energy of a conjugated hydrocarbon, as calculated with the "Hückel molecular orbital (HMO) method," coincides with the energy (as we are going to define below) of the corresponding graph. Conjugated hydrocarbons are of great importance for science and technology. A *conjugated hydrocarbon* can be characterized as a molecule composed entirely of carbon and hydrogen atoms in which every carbon atom has exactly three neighbors (which are either carbon or hydrogen atoms). See Fig. 11.3, which gives the structure of butadiene.

The graph corresponding to a conjugated hydrocarbon is taken as follows (which is somewhat different from our description of molecular graphs given earlier in Chap. 1, and there are valid theoretical reasons for doing this): Every carbon atom is represented by a vertex and every carbon–carbon bond by an edge. Hydrogen atoms are ignored. Thus, the graph for the molecule of Fig. 11.3 is the path P_4 on four vertices. These graphs of the conjugated hydrocarbons are connected and their vertex degrees are at most 3. However, for our general definition of graph energy, there is no such restriction and our graphs are quite general—only, they are simple.

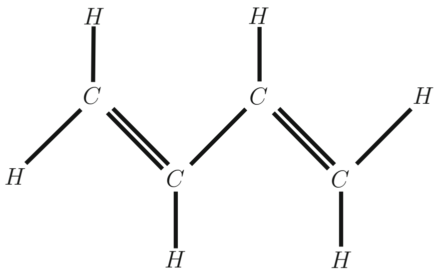


Fig. 11.3 Butadiene

The pioneer in this area is Ivan Gutman. Readers interested in doing research in graph energy should consult [82, 83, 84].

Definition 11.12.1. The *energy* of a graph G is the sum of the absolute values of its eigenvalues.

Hence if $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of a graph G of order n, the energy $\mathcal{E}(G)$ of G is given by

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|.$$

Example 11.12.2. 1. The energy of the complete graph $K_n = \mathcal{E}(K_n) = (n-1) + (n-1)|-1| = 2(n-1)$.

2. The spectrum of the Petersen graph is $\begin{pmatrix} 3 & 1 & -2 \\ 1 & 5 & 4 \end{pmatrix}$. (See Exercise 14.14). Hence, its energy is $1.3 + 5.1 + 4.2 = 16$.

11.12.2 Maximum Energy of k-Regular Graphs

Theorem 11.12.3. *The maximum energy of a k-regular graph G of order n is $k + \sqrt{k(n-1)(n-k)}$.*

Proof. Let $Sp(G) = \{\lambda_1 = k, \lambda_2, \ldots, \lambda_n\}$. Apply Cauchy–Schwarz's inequality to the two vectors $(|\lambda_2|, |\lambda_3|, \ldots, |\lambda_n|)$ and $(1, 1, \ldots, 1)$. This gives

$$\left(\sum_{i=2}^{n} |\lambda_i|.1\right)^2 \leq \left(\sum_{i=2}^{n} |\lambda_i|^2\right)\left(\sum_{i=2}^{n} 1^2\right)$$

so that (as $\sum_{i=1}^{n} \lambda_i^2 = 2m$)

$$\big(\mathcal{E}(G) - \lambda_1\big) \leq \sqrt{(2m - \lambda_1^2)(n-1)}.$$

Therefore, $\mathcal{E}(G) \le F(\lambda_1)$, where

$$F(\lambda_1) := \lambda_1 + \sqrt{(2m - \lambda_1^2)(n-1)}. \tag{11.17}$$

If G is k-regular, by Theorem 11.5.1, $\lambda_1 = k$, and hence

$$\begin{aligned}\mathcal{E}(G) &\le k + \sqrt{(n-1)(2m-k^2)} \\ &= k + \sqrt{k(n-1)(n-k)} \quad (\text{as } 2m = nk).\end{aligned} \tag{11.18}$$

□

The same method yields for a general (not necessarily regular) graph the following theorem of Gutman [84].

Theorem 11.12.4. *Let G be a graph of order n and size m. Then*

$$\mathcal{E}(G) \le \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]}. \tag{11.19}$$

Proof. As usual, let A stand for the adjacency matrix of G. We have

$$\sqrt{\frac{2m}{n}} \le \frac{2m}{n} \le \lambda_1 \le \sqrt{2m}. \tag{11.20}$$

Relation (11.20) is a consequence of the fact that $0 < \lambda_1^2 \le \lambda_1^2 + \cdots + \lambda_n^2 = 2m$ and Exercise 14.10. Moreover, by (11.17), $\mathcal{E}(G) \le F(\lambda_1)$. Now the function $F(x) = x + \sqrt{(n-1)(2m-x^2)}$ is strictly decreasing in the interval $\sqrt{\frac{2m}{n}} < x \le \sqrt{2m}$. Hence, by inequality (11.20),

$$\mathcal{E}(G) \le F(\lambda_1) \le F\left(\frac{2m}{n}\right) = \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]}. \tag{11.21}$$

□

Theorem 11.12.5. *If $2m \ge n$ and G is a graph on n vertices and m edges, then $\mathcal{E}(G) = \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]}$ if and only if G is either $\frac{n}{2}K_2$, K_n or a non-complete connected strongly regular graph for which the spectrum $\{\lambda_1 > \lambda_2 \ge \ldots \ge \lambda_n\}$ has the property that $|\lambda_2| = |\lambda_3| = \ldots = |\lambda_n| = \sqrt{\frac{2m - \left(\frac{2m}{n}\right)^2}{n-1}}$.*

Proof. We have already seen in Theorem 11.12.4 that $\mathcal{E}(G) \le F\left(\frac{2m}{n}\right) = \frac{2m}{n} + \sqrt{(n-1)\left(2m - \left(\frac{2m}{n}\right)^2\right)}$. If $G \simeq \frac{n}{2}K_2$, then $Sp(G) = \begin{pmatrix} 1 & -1 \\ \frac{n}{2} & \frac{n}{2} \end{pmatrix}$, and if $G \simeq K_n$, then $Sp(K_n) = \begin{pmatrix} 1 & -1 \\ 1 & n-1 \end{pmatrix}$. In both cases, it is routine to check that $\mathcal{E}(G) = F(\frac{2m}{n})$.

If the third alternative holds, G is regular of degree (see Theorem 11.5.1) $\frac{2m}{n} = \lambda_1$, and hence $\mathcal{E}(G)$, which, by hypothesis, is equal to $\lambda_1 + (n-1)\sqrt{\frac{2m-\left[\frac{2m}{n}\right]^2}{n-1}} = \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]} = F\left(\frac{2m}{n}\right)$, and therefore equality holds in (11.19).

Conversely, assume that equality is attained in (11.19) for some graph G. Then (11.20) and (11.21) together with the strict decreasing nature of $F(x)$ imply that λ_1 (maximum degree of G) $= \frac{2m}{n}$ (average degree of G). Hence, G must be regular of degree $\frac{2m}{n}$. Moreover, in this case, equality must be attained in the Cauchy–Schwarz inequality applied in the proof of Theorem 11.12.3 and hence $(|\lambda_2|, \ldots, |\lambda_n|)$ is a scalar multiple of $(1, 1, \ldots, 1)$. In other words, $|\lambda_2| = \ldots = |\lambda_n|$. Consequently, $|\lambda_2| + \cdots + |\lambda_n| = (n-1)|\lambda_i| = \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]}$, and therefore, $|\lambda_i| = \sqrt{\frac{\left[2m-\left(\frac{2m}{n}\right)^2\right]}{n-1}}$, $2 \le i \le n$. This results in three cases.

Case (i). The graph G has two distinct eigenvalues λ_1 and λ_2 with $|\lambda_1| = |\lambda_2|$. [If all the eigenvalues of G are equal, they must all be zero (as $\sum \lambda_i = 0$) and hence G must be the totally disconnected graph K_n^c.] Let m_1 and m_2 be the multiplicities of λ_1 and λ_2, respectively. Then $0 = tr(A) = m_1\lambda_1 + m_2\lambda_2$ and hence $m_1 = m_2$. This gives $\lambda_2 = -\lambda_1$, and therefore $\lambda_2 = -\sqrt{\frac{\left[2m-\left(\frac{2m}{n}\right)^2\right]}{n-1}} = -\lambda_1 = -\frac{2m}{n}$, which reduces to $n = 2m$. If G has ω components, $\frac{n}{2} = m \ge n-\omega$, and hence $\omega \ge \frac{n}{2}$. As G has no isolated vertices, $\omega = \frac{n}{2}$, and hence $G \simeq \frac{n}{2}K_2$.

Case (ii). G has two eigenvalues with distinct absolute values. Then $|\lambda_1| \ne |\lambda_2| (= |\lambda_3| = \ldots = |\lambda_n|)$. Now $tr(A) = 0$ gives $\frac{2m}{n} + (n-1)\sqrt{\frac{\left[2m-\left(\frac{2m}{n}\right)^2\right]}{n-1}} = 0$, which gives, on simplification, $m = \frac{n(n-1)}{2}$. Hence, $G \simeq K_n$.

Case (iii). G has exactly three distinct eigenvalues with distinct absolute values equal to $\frac{2m}{n}$ and $\sqrt{\frac{\left[2m-\left(\frac{2m}{n}\right)^2\right]}{n-1}}$.

The conclusion in this case is an immediate consequence of a result of Shrikhande and Bhagwandas [172], which states that a k-regular connected graph G of order n is strongly regular if and only if it has three distinct eigenvalues $\alpha_1 = k, \alpha_2, \alpha_3$ and if G is an $srg(n, k, \lambda, \mu)$, then $\lambda = k + \alpha_2\alpha_3 + \alpha_2 + \alpha_3$, and $\mu = k + \alpha_2\alpha_3$. Hence, G must be connected (as the multiplicity of k is 1) and strongly regular. □

Remark 11.12.6. Theorems 11.12.4 and 11.12.5 deal with the case $2m \ge n$. If $2m < n$, the graph G is disconnected with $n - 2m$ isolated vertices. Removal of these isolated vertices from G results in a subgraph G' of G with $n' = 2m$ vertices and hence $G' \simeq mK_2$ by Theorem 11.12.5. Therefore, in this case, $G \simeq mK_2 \cup K_{n-2m}^c$.

We conclude this section with the theorem of Koolen and Moulton [124] on the characterization of maximum energy graphs with a given number n of vertices.

Theorem 11.12.7. *Let G be a graph on n vertices. Then $\mathcal{E}(G) \le \frac{n}{2}(1+\sqrt{n})$ with equality holding if and only if G is a strongly regular graph with parameters $(n, \frac{n+\sqrt{n}}{2}, \frac{n+2\sqrt{n}}{4}, \frac{n+2\sqrt{n}}{4})$.*

Proof. First, assume that $2m \ge n$. By Theorem 11.12.4,

$$\mathcal{E}(G) \le F(m) = \frac{2m}{n} + \sqrt{(n-1)\Big[2m - \Big(\frac{2m}{n}\Big)^2\Big]}. \qquad (11.22)$$

We are interested in finding the values of m for which $F(m)$ attains the maximum. This is done by the methods of elementary calculus: $F'(m) = 0$ gives $16nm^2 - 8n^3m + (n^5 - n^4) = 0$, and this is the case when $m = \frac{n^2 \pm n\sqrt{n}}{4}$. Further, $F''(m) < 0$ only for $m = \frac{n^2+n\sqrt{n}}{4}$. Hence, $f(m)$ attains its maximum when $m = \frac{n^2+n\sqrt{n}}{4}$, and for this value of m, $F(\frac{2m}{n}) = F(\frac{n+\sqrt{n}}{2}) = \frac{n^3+\sqrt{n}}{2}$.

Next, assume that G is a strongly regular graph with parameters given in Theorem 11.12.5. As G is k-regular with $k = \frac{n+\sqrt{n}}{2}$, by Theorem 11.12.3,

$$\begin{aligned}\mathcal{E}(G) &= k + \sqrt{k(n-1)(n-k)} \\ &= \frac{n+\sqrt{n}}{2} + \sqrt{\left(\frac{n+\sqrt{n}}{2}\right)(n-1)\left(n - \frac{n+\sqrt{n}}{2}\right)} \\ &= \frac{n^{3/2}+n}{2}, \text{ the maximum possible energy.}\end{aligned}$$

Finally, assume that G attains the maximum possible energy. We have to show that G is an $srg(n, \frac{n+\sqrt{n}}{2}, \frac{n+2\sqrt{n}}{4}, \frac{n+2\sqrt{n}}{4})$. By Theorem 11.12.5, three cases arise:

Case (i). $\frac{n(1+\sqrt{n})}{2} = \mathcal{E}(G) = \mathcal{E}(\frac{n}{2}K_2) = n$. This case cannot arise (as $n > 1$).

Case (ii). $\frac{n(1+\sqrt{n})}{2} = \mathcal{E}(G) = \mathcal{E}(K_n) = 2(n-1)$. This gives $(n-1)(n-4)^2 = 0$ and hence $G \simeq K_4$, and corresponds to a degenerate strongly regular graph.

Case (iii). G is a strongly regular graph with two eigenvalues λ_2 and λ_3 (distinct from $\lambda_1 = \frac{2m}{n}$) both having the same absolute value $\sqrt{\frac{\left[2m - \left(\frac{2m}{n}\right)^2\right]}{n-1}}$.

Recall that λ_2 and λ_3 are the roots of the quadratic equation (see (11.10) of Theorem 11.10.5) $x^2 + (\mu - \lambda)x + (\mu - k) = 0$, where $k = \lambda_1 = \frac{2m}{n}$. Now $\lambda_2 + \lambda_3 = 0$ gives $\lambda = \mu$. Moreover, $\lambda_2\lambda_3 = \mu - k$ gives $\mu - \frac{2m}{n} = \lambda_2\lambda_3 = -\left(\frac{2m - (\frac{2m}{n})^2}{n-1}\right)$. Substituting $m = \frac{nk}{2} = n\frac{n(n+\sqrt{n})}{2}$ and simplifying, we get $\mu = \frac{n+2\sqrt{n}}{4} = \lambda$. Hence, G is strongly regular with parameters $(n, \frac{n+\sqrt{n}}{2}, \frac{n+2\sqrt{n}}{4}, \frac{n+2\sqrt{n}}{4})$. □

Finally, if $2m < n$, by Remark 11.12.6, $\mathcal{E}(G) \le 2m < n < \frac{n(1+\sqrt{n})}{2}$, $n \ge 1$. Hence, the case $2m = \frac{n(1+\sqrt{n})}{2}$ cannot arise.

11.12.3 Hyperenergetic Graphs

The complete graph K_n, as seen in Example 11.12.2, has energy $2(n-1)$. It was conjectured by Gutman [82] that if G is any graph of order n, then $\mathcal{E}(G) \leq 2(n-1) = \mathcal{E}(K_n)$. This was disproved by many: Gutman et al. in [86] and Walikar et al. in [189]. Graphs G of order n for which $\mathcal{E}(G) > 2(n-1)$ have been called *hyperenergetic graphs.*

Example 11.12.8. (i) K_n is nonhyperenergetic.

(ii) All cubic graphs are nonhyperenergetic. If G is cubic, $k = 3$. Hence, by Theorem 11.12.3, $\mathcal{E}(G) \leq 3 + \sqrt{3(n-1)(n-3)}$. Now, $3 + \sqrt{3(n-1)(n-3)} \leq 2(n-1)$ if and only if $n^2 - 8n + 16 \geq 0$, which is true as $n \geq 4$ for any cubic graph.

(iii) If $n \geq 5$, $L(K_n)$ is hyperenergetic.

(iv) If $n \geq 4$, $L(K_{n,n})$ is hyperenergetic.

We leave the proofs of (iii) and (iv) as exercises (See [188]).

Theorem 11.12.9 (Stevanović and Stanković [173]). *The graph $K_n - H$, where H is a Hamilton cycle of K_n, $n \geq 10$ is hyperenergetic.*

Proof. Let $H = (v_1 v_2 \dots v_n)$. Then the adjacency matrix A of $K_n - H$ is a circulant with first row (0 0 1 1 ... 1 0). Hence, by Lemma 11.2.3,

$$Sp(K_n - H) = \{\omega^{2r} + \omega^{3r} + \cdots + \omega^{(n-2)r} \,:\, \omega = \text{a primitive } n\text{th root of unity}\}.$$

$$= \begin{cases} n-3, & \text{if } \omega = 1 \\ -1 - \omega^r - \omega^{r(n-1)}, & \text{if } \omega \neq 1,\ 1 \leq r \leq n-1. \end{cases}$$

$$= \begin{cases} n-3, & \text{if } \omega = 1 \\ -1 - 2\cos\frac{2\pi r}{n}, & \text{if } \omega \neq 1,\ 1 \leq r \leq n-1. \end{cases}$$

Hence, $\mathcal{E}(K_n - H) = (n-3) + \sum_{r=1}^{n-1} \left| -1 - 2\cos\frac{2\pi r}{n} \right|$, which shows that (by the definition of Riemann integral) $\mathcal{E}(K_n - H) \to (n-3) + \frac{n-1}{2\pi} \int_0^{2\pi} \left| -1 - 2\cos x \right| \mathrm{d}x$ as $n \to \infty$.

Hence,

$$\lim_{n\to\infty} \frac{\mathcal{E}(K_n - H)}{n-1} = 1 + \frac{1}{2\pi} \int_0^{2\pi} \left| -1 - 2\cos x \right| \mathrm{d}x$$
$$= \frac{4\sqrt{3}}{2\pi} + \frac{1}{3}$$
$$\approx 2.43599,$$

which shows that there exists n_0 such that for $n \geq n_0$, $\mathcal{E}(K_n - H) > 2(n-1)$. Computations show that $n_0 = 10$. ☐

Theorem 11.12.9 disproves a conjecture given in [10].

Graph $\overline{C}(n; k_1, \ldots, k_r)$, $k_1 < k_2 < \ldots < k_r < \frac{n}{2}$, $k_i \in \mathbb{N}$ for each i is the circulant graph with vertex set $V = \{0, 1, \ldots, n-1\}$ such that a vertex u is adjacent to all the vertices of $V \backslash \{u\}$, except $u \pm k_i \,(\mathrm{mod}\, n)$, $i = 1, 2, \ldots, n$. Note that $K_n - H$ is just $\overline{C}(n; 1)$. Stevanović and Stanković also generalized Theorem 11.12.9 as follows:

Theorem 11.12.10 (Stevanović and Stanković [173]). *Given $k_1 < k_2 < \ldots < k_r$, there exists $n_0 \in \mathbb{N}$ such that for $n \geq n_0$, the graph $\overline{C}(n; k_1, \ldots, k_r)$ is hyperenergetic.*

11.12.4 Energy of Cayley Graphs

We now compute the energy of the unitary Cayley graph X_{p^α}, where p is a prime. This can be done in two ways: In [10], Balakrishnan computed it using cyclotomic polynomials, while in [161], Ramaswamy and Veena computed it using Ramanujan sums. We present the latter method.

Theorem 11.12.11. *If p is a prime and $r \geq 1$, $\mathcal{E}(X_{p^\alpha}) = 2\phi(p^\alpha)$.*

Proof. If $\alpha = 1$, $X_{p^\alpha} = X^p = K_p$, and $\mathcal{E}(K_p) = 2(p-1) = 2\phi(p)$. So assume that $\alpha \geq 2$. By Theorem 11.9.2, $Sp(X_{p^\alpha}) = \{\lambda_0, \ldots, \lambda_{n-1}\}$, where

$$\lambda_{r+1} = c(r, p^\alpha) = \mu(t_r)\frac{\phi(p^\alpha)}{\phi(t_r)}, \text{ and } t_r = \frac{p^\alpha}{(r, p^\alpha)}, \; 0 \leq r < p^\alpha.$$

Here μ is the Möebius function and ϕ is Euler's totient function.

We consider three cases:

(i) $(r, p^\alpha) = p^\alpha$. Then as $r < p^\alpha$, $r = 0$, $t_r = 1$, and $\mu(t_r) = 1$, and therefore $\lambda_1 = \frac{\phi(p^\alpha)}{\phi(1)} = p^\alpha - p^{\alpha-1}$.

(ii) $(r, p^\alpha) = 1$. Then $t_r = p^\alpha$ and therefore $\mu(t_r) = 0$. Hence, $\lambda_{r+1} = 0$ in this case.

(iii) If $1 < (r, p^\alpha) < p^\alpha$, then $(r, p^\alpha) = p^m$, $1 \leq m \leq \alpha - 1$. If $(r, p^\alpha) = p^{\alpha-1}$, then $r \in \{1.p^{\alpha-1}, 2.p^{\alpha-1}, \ldots, (p-1).p^{\alpha-1}\}$, and hence $t_r = p$ and therefore $\mu(t_r) = -1$. Hence, $\lambda_{r+1} = -\frac{\phi(p^\alpha)}{\phi(p)} = -p^{\alpha-1}$.

In all the other cases, $\mu(t_r) = 0$, and therefore $\lambda_{r+1} = 0$.

Hence, $Sp(X_{p^\alpha}) = \begin{pmatrix} p^\alpha - p^{\alpha-1} & -p^{\alpha-1} & 0 \\ 1 & p-1 & p^\alpha - p \end{pmatrix}$, and therefore

$$\begin{aligned} \mathcal{E}(X_{p^\alpha}) &= (p^\alpha - p^{\alpha-1}) + (p-1)p^{\alpha-1} \\ &= 2(p^\alpha - p^{\alpha-1}) \\ &= 2\phi(p^\alpha). \end{aligned}$$

□

In [10], Theorem 11.12.11 has been applied to prove the next result, which in essence constructs for each n, a k-regular graph of order n for a suitable k whose energy is small compared to the maximum possible energy among the class of k-regular graphs.

Theorem 11.12.12 ([10]). *For each $\epsilon > 0$, there exist infinitely many n for each of which there exists a k-regular graph G of order n with $k < n-1$ and $\frac{\mathcal{E}(G)}{B} < \epsilon$, where B is the maximum energy that a k-regular graph on n vertices can attain.*

Proof. The Cayley graph X_{p^α} is $\phi(p^\alpha)$-regular. The maximum energy that a k-regular graph can attain is (by Theorem 11.12.3) $B = k + \sqrt{k(n-1)(n-k)}$. Taking $n = p^\alpha$ and $k = \phi(p^\alpha)$, this bound becomes

$$\begin{aligned} B &= \phi(p^\alpha) + \sqrt{\phi(p^\alpha)(p^\alpha - 1)(p^\alpha - \phi(p^\alpha))} \\ &= (p^\alpha - p^{\alpha-1}) + \sqrt{(p^\alpha - p^{\alpha-1})(p^\alpha - 1)p^{\alpha-1}} \\ &= (p^\alpha - p^{\alpha-1}) + p^{\alpha-1}\sqrt{(p-1)(p^\alpha - 1)}. \end{aligned}$$

Hence, $$\frac{\mathcal{E}(X_{p^\alpha})}{B} = \frac{2(p^\alpha - p^{\alpha-1})}{(p^\alpha - p^{\alpha-1}) + p^{\alpha-1}\sqrt{(p-1)(p^\alpha-1)}} = \frac{2}{1 + \sqrt{1 + p + \cdots + p^{\alpha-1}}} \longrightarrow 0 \text{ as either } p \to \infty \text{ or } \alpha \to \infty.$$

□

In [10], the following dual question was also raised: Given a positive integer $n \geq 3$, and $\epsilon > 0$, does there exist a k-regular graph G of order n such that $\frac{\mathcal{E}(G)}{B} > 1 - \epsilon$ for some $k < (n-1)$? An affirmative answer to this question is given in [133] and [190], not for general n, but when n is a prime power $p^m \equiv 1 (\text{mod } 4)$. Interestingly, both papers give the same example, namely, the Paley graph [see Example 11.10.2(v)].

Lemma 11.12.13. $\mathcal{E}(G_1 \times G_2) = \mathcal{E}(G_1)\mathcal{E}(G_2)$.

Proof. From Corollary 11.8.7, it follows that if $Sp(G_1) = \{\lambda_1, \ldots, \lambda_p\}$ and $Sp(G_2) = \{\mu_1, \ldots, \mu_q\}$, then $Sp(G_1 \times G_2) = \{\lambda_i \mu_j : 1 \leq i \leq p, 1 \leq j \leq q\}$. Hence,

$$\mathcal{E}(G_1 \times G_2) = \sum_{i=1}^{p}\sum_{j=1}^{q} |\lambda_i \mu_j| = \Big(\sum_{i=1}^{p} |\lambda_i|\Big)\Big(\sum_{j=1}^{q} |\mu_j|\Big) = \mathcal{E}(G_1)\mathcal{E}_(G_2).$$ □

Recall Theorem 11.9.2, which states that if $(n_1, n_2) = 1$, $X_{n_1 n_2} \simeq X_{n_1} \times X_{n_2}$.

Corollary 11.12.14 ([161]). $\mathcal{E}(X_n) = 2^k \phi(n)$, *where k is the number of distinct prime factors of n.*

Proof. If p_1 and p_2 are distinct primes, then by Lemma 11.12.13, $\mathcal{E}(X_{p_1^{\alpha_1} p_2^{\alpha_2}}) = \mathcal{E}(X_{p_1^{\alpha_1}})\mathcal{E}(X_{p_2^{\alpha_2}}) = 2\phi(p_1^{\alpha_1}).2\phi(p_2^{\alpha_2}) = 2^2\phi(p_1^{\alpha_1} p_2^{\alpha_2})$. By induction, it follows that if $n = p_1^{\alpha_1} \dots p_k^{\alpha_k}$, where the p_i's are the distinct prime factors of n, $\mathcal{E}(X_n) = \prod_{i=1}^{k} \mathcal{E}(p_i^{\alpha_i}) = \prod_{i=1}^{k} 2\phi(p_i^{\alpha_i}) = 2^k \phi(n)$. □

The last result has also been proved in [108] using different techniques.

11.13 Energy of the Mycielskian of a Regular Graph

In this section we determine the energy of the Mycielskian of a k-regular graph G in terms of the energy of G. [We defined the Mycielskian $\mu(G)$ of a graph G in Chap. 7.] Some papers that deal with the energy of regular graphs are [4, 87, 109].

Theorem 11.13.1 ([13]). *Let G be a k-regular graph on n vertices. Then the energy $\mathcal{E}(\mu(G))$ of $\mu(G)$ is given by*

$$\mathcal{E}(\mu(G)) = \sqrt{5}\mathcal{E}(G) - (\sqrt{5} - 1)k + 2|t_3|, \tag{11.23}$$

where $\mathcal{E}(G)$ is the energy of G and t_3 is the unique negative root of the cubic

$$t^3 - kt^2 - (n + k^2)t + kn. \tag{11.24}$$

Proof. Denote by A the adjacency matrix of G. As A is real symmetric, $A = PDP^{\mathrm{T}}$, where D is the diagonal matrix diag$(\lambda_1, \dots, \lambda_n)$, and P is an orthogonal matrix with orthonormal eigenvectors p_i's, that is, $Ap_i = \lambda_i p_i$ for each i. In particular, if e denotes the n-vector with all entries equal to 1, then $p_1 = \frac{e}{\sqrt{n}}$ (G being regular). Hence, $e^{\mathrm{T}} p_i$=0 for $i = 2, \dots, n$, and consequently $e^{\mathrm{T}} P = [\sqrt{n}, 0, \dots, 0]$.

Now, by the definition of $\mu(G)$, the adjacency matrix of $\mu(G)$ is the matrix of order $(2n + 1)$ given by

$$\mu(A) = \begin{bmatrix} A & A & 0 \\ A & 0 & e \\ 0 & 0e^{\mathrm{T}} & 0 \end{bmatrix}.$$

Since $A = PDP^{\mathrm{T}}$, we have

$$\mu(A) = \begin{bmatrix} PDP^{\mathrm{T}} & PDP^{\mathrm{T}} & 0 \\ PDP^{\mathrm{T}} & 0 & e \\ 0 & e^{\mathrm{T}} & 0 \end{bmatrix}$$
$$= \begin{bmatrix} P & 0 & 0 \\ 0 & P & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} D & D & 0 \\ D & 0 & P^{\mathrm{T}}e \\ 0 & e^{\mathrm{T}}P & 0 \end{bmatrix} \begin{bmatrix} P^{\mathrm{T}} & 0 & 0 \\ 0 & P^{\mathrm{T}} & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

As P is an orthogonal matrix, the spectrum of $\mu(A)$ is the same as the spectrum of

$$B = \begin{bmatrix} D & D & 0 \\ D & 0 & [\sqrt{n}, 0, \ldots, 0]^{\mathrm{T}} \\ 0 & [\sqrt{n}, 0, \ldots, 0] & 0 \end{bmatrix}.$$

The determinant of the characteristic matrix of B is given by

$$\left|\begin{array}{cccc:cccc:c} x-\lambda_1 & & & 0 & -\lambda_1 & & & 0 & 0 \\ & x-\lambda_2 & & & & -\lambda_2 & & & 0 \\ & & \ddots & & & & \ddots & & \vdots \\ 0 & & & x-\lambda_n & 0 & & & -\lambda_n & 0 \\ \hdashline -\lambda_1 & & & 0 & x & & & 0 & -\sqrt{n} \\ & -\lambda_2 & & & & x & & & 0 \\ & & \ddots & & & & \ddots & & \vdots \\ 0 & & & -\lambda_n & 0 & & & x & 0 \\ \hdashline 0 & 0 & \cdots & 0 & -\sqrt{n} & 0 & \cdots & 0 & x \end{array}\right|.$$

We now expand $\det(xI - B)$ along its first, $(n+1)$th, and $(2n+1)$th columns by Laplace's method [61]. [Recall that Laplace's method of expansion of a determinant T along any chosen set $\{C_{j_1}, \ldots, C_{j_k}\}$ of k columns (or rows) is a natural generalization of the usual expansion of a determinant along any column (or row). This expansion of T is given by $\sum_{(i_1,\ldots,i_k)} (-1)^{(i_1+\cdots+i_k)+(j_1+\cdots+j_k)} U_k V_{2n+1-k}$, where U_k is the determinant minor of T of order k common to the k rows $R_{i_1}, \ldots, R_{i_k}$, and the k columns $C_{j_1}, \ldots, C_{j_k}$, and V_{2n+1-k} is the complementary determinant minor of order $(2n+1-k)$ obtained by deleting these sets of k rows and k columns from T.] In this expansion, only the 3×3 minor, which is common to the above three columns, and the 1-st, $(n+1)$th, and $(2n+1)$th rows are nonzero. This minor is

$$M_1 = \begin{vmatrix} x-\lambda_1 & -\lambda_1 & 0 \\ -\lambda_1 & 0 & -\sqrt{n} \\ 0 & -\sqrt{n} & 0 \end{vmatrix}.$$

We now expand the complementary minor of M_1 along the 2nd and $(n+2)$th columns, and then the resulting complementary minor by the 3rd and $(n+3)$th columns, and so on. These expansions give the spectrum of $\mu(A)$ to be the union of the spectra of the matrices

$$\begin{bmatrix} \lambda_1 & \lambda_1 & 0 \\ \lambda_1 & 0 & \sqrt{n} \\ 0 & \sqrt{n} & 0 \end{bmatrix}, \begin{bmatrix} \lambda_2 & \lambda_2 \\ \lambda_2 & 0 \end{bmatrix}, \ldots, \begin{bmatrix} \lambda_n & \lambda_n \\ \lambda_n & 0 \end{bmatrix}.$$

(Another way to see this is to observe that B is orthogonally similar to the direct sum of the above n matrices.) Thus, the spectrum of $\mu(A)$ is

$$\left\{t_1,\, t_2,\, t_3,\, \lambda_2\left(\frac{1\pm\sqrt{5}}{2}\right), \ldots, \lambda_n\left(\frac{1\pm\sqrt{5}}{2}\right)\right\},$$

where t_1, t_2, t_3 are the roots of the cubic polynomial $t^3 - kt^2 - (n+k^2)t + kn$ (note that as G is k-regular, $\lambda_1 = k$), which has two positive roots and one negative root, say, $t_1 > t_2 > 0 > t_3$.

Let $\mathcal{E}(G)$ denote the energy of G. Then $\mathcal{E}(G) = \sum_i |\lambda_i| = k + |\lambda_2| + \cdots + |\lambda_n|$. Hence, the energy of the Mycielskian $\mu(G)$ of G, when G is k-regular, is

$$\begin{aligned}\mathcal{E}(\mu(G)) &= |t_1| + |t_2| + |t_3| + \big(|\frac{1+\sqrt{5}}{2}| + |\frac{1-\sqrt{5}}{2}|\big)\big(|\lambda_2| + \cdots + |\lambda_n|\big)\\ &= t_1 + t_2 + |t_3| + \sqrt{5}(|\lambda_2| + \cdots + |\lambda_n|)\\ &= k - t_3 + |t_3| + \sqrt{5}(\mathcal{E}(G) - k)\\ &= \sqrt{5}\mathcal{E}(G) - (\sqrt{5}-1)k + 2|t_3|.\end{aligned}$$

□

11.13.1 An Application of Theorem 11.13.1

We have shown in Theorem 11.12.7 that the maximum energy that a graph G of order n can have is $\frac{n^{\frac{3}{2}}+n}{2}$ and that G has maximum energy if and only if it is a strongly regular graph with parameters $\left(n, \frac{n+\sqrt{n}}{2}, \frac{n+2\sqrt{n}}{4}, \frac{n+2\sqrt{n}}{4}\right)$. If $n > 25$ and G has maximum energy, $\mathcal{E}(G) > 3n > 2(n-1)$ and hence G is hyperenergetic. Also, from (11.23), $\mathcal{E}(\mu(G)) > 3n\sqrt{(5)} - (\sqrt{(5)} - 1)k + 2|t_3| > 3n\sqrt{(5)} - (\sqrt{(5)} - 1)(n-1) > 2\sqrt{(5)}n + \sqrt{(5)} + 1 > 4n = 2[(2n+1)-1]$. Hence, the Mycielskians of maximal energy graphs of order $n > 25$ are all hyperenergetic. More generally, if G is a regular graph of order n and $\mathcal{E}(G) > 3n$, then $\mu(G)$ is hyperenergetic.

Example 11.13.2 ([13]). We now present two examples. Consider two familiar regular graphs, namely, the Petersen graph P and a unitary Cayley graph.

1. For P, $n = 10$, $m = 15$, and $k = 3$. The spectrum of P is $\begin{pmatrix} 3 & 1 & -2 \\ 1 & 5 & 4 \end{pmatrix}$. Hence, $\mathcal{E}(P) = 16$. Now for P, the polynomial (3.2) is $t^3 - 3t^2 - 19t + 30$, and its unique negative root t_3 is ≈ -3.8829. Hence, from (11.23), $\mathcal{E}(\mu(P)) \approx 16\sqrt{5} - (\sqrt{5}-1)3 + 2(3.8829) = 39.8347 < 40 = 2(21-1)$, where 21 is the order of $\mu(P)$. Hence, $\mu(P)$ is non-hyperenergetic.
2. Consider the unitary Cayley graph $G = \mathrm{Cay}(\mathbb{Z}_{210}, U)$, U being the group of multiplicative units of the additive group $(\mathbb{Z}_{210}, +)$. Then $\mathcal{E}(G) = 2^4\phi(210) = 768 > 3 \times 210 = 3n$. Here $n = 210$, $k = \phi(210) = 48$. Hence, the polynomial

(11.24) becomes $t^3 - 48t^2 - 2514t + 10,080$, for which the unique negative root t_3 is ≈ -34.18. Hence, from (11.23), $\mathcal{E}(\mu(G)) \approx 768\sqrt{5} - (\sqrt{5} - 1)$ $48 + 2(34.18) = 1,726.352 > 2((2n + 1) - 1) = 840$. Thus, $\mu(\text{Cay}(\mathbb{Z}_{210}, U))$ is hyperenergetic, as expected.

11.14 Exercises

14.1. Prove: For any nontrivial graph of order n with spectrum $= \{\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n\}$, $\lambda_n \leq 0$.

14.2. If G is k-regular, show that the number of connected components of G is the multiplicity of k as an eigenvalue of G.

14.3. Prove by induction on l that the number of v_i-v_j walks of length l in the connected graph G with $V(G) = \{v_1, \ldots, v_n\}$ is the (i, j)th entry of A^l. Hence show that the diameter of a connected graph G is the least positive integer d with $A^d > 0$ (that is, all the entries of A^d are positive).

14.4. Let G be a complete r-partite graph of order n with all parts of the same size. Find $Sp(G)$. In particular, find $Sp(K_{p,p})$, and compare it with Theorem 11.6.1.

14.5. If G and H are disjoint graphs, prove that $Sp(G \cup H) = Sp(G) \cup Sp(H)$, and that $\phi(G \cup H; \lambda) = \phi(G; \lambda)\phi(H; \lambda)$.

14.6. The Möbius ladder M_h is the cubic graph obtained by joining the opposite vertices of the cycle C_{2h}. Show that the spectrum of the Möbius ladder is given by $\lambda_j = 2\cos\frac{\pi j}{h} + (-1)^j$, $0 \leq j \leq 2h - 1$.

14.7. Find the spectrum of

(i) $C_4 \times C_3$,

(ii) $K_4 \Box K_3$,

(iii) $L(K_{4,3})$ using Sachs' theorem and hence comment on the results in (ii) and (iii).

14.8. If G is a bipartite graph of odd order, prove that det A is zero.

14.9. If G is bipartite and A is nonsingular, show that G has a perfect matching.

14.10. Let G be a graph of order n with adjacency matrix A. Prove that for any nonzero vector $\mathbf{x} \in \mathbb{R}^n$, $\lambda_1 = \lambda_{\max}(G) \geq \frac{(A\mathbf{x},\mathbf{x})}{(\mathbf{x},\mathbf{x})} \geq \lambda_{\min}(G) = \lambda_n$. In particular, show that $\lambda_1 \geq \frac{2m}{n}$. (Hint: Use the fact that $\mathbb{R}^n$ has an orthonormal basis of eigenvectors of A.)

14.11. Find the spectrum of $K_4 \boxtimes K_3$.

14.12. Show that a graph G on n vertices is connected if and only if each entry of $(A + I)^{n-1}$ is positive.

14.13. Let $\lambda_1, \ldots, \lambda_r$ be the distinct eigenvalues of A, the adjacency matrix of a graph G of order n. Prove that the minimal polynomial of A is $(x - \lambda_1) \ldots (x - \lambda_r)$. (Hint: Same as for Exercise 14.10.)

14.14. Using the fact that the Petersen graph $P \simeq (L(K_5))^c$, show that $Sp(P) = \begin{pmatrix} 3 & 1 & -2 \\ 1 & 5 & 4 \end{pmatrix}$.
14.15. Is the Petersen graph a Cayley graph?
14.16. When n is a prime, show that the unitary Cayley graph X_n is the complete graph K_n.
14.17. Let G be a finite abelian group of order n. Prove that $Sp\big(\mathrm{Cay}(G;S)\big) = \{\lambda_\chi = \sum_{s \in S} \chi(s) \,:\, \chi =$ an irreducible character of $G\}$. [Hint: Show that if $G = \{g_1, \ldots, g_n\}$, then $\big(\chi(g_1), \ldots, \chi(g_n)\big)^{\mathrm{T}}$ is an eigenvector of the adjacency matrix of the Cayley graph.]
14.18. If λ is any eigenvalue of a graph G of order n and size m, prove that $\lambda \le \sqrt{\frac{2m}{n}(n-1)}$. (Hint: Imitate the relevant steps given in the proof of Theorem 11.12.3.)
14.19. Show that the Petersen graph is a Ramanujan graph.
14.20. Show that the graphs $K_n \times K_n \times \ldots \times K_n$ p times, where $p \ge 4$, $n \ge 3$, form a family of regular graphs none of which is a Ramanujan graph.
14.21. Prove that if G is bipartite, then $\chi(G;x)$ is of the form $\phi(x^2)$ or $x\phi(x^2)$. Hence, prove that if λ is an eigenvalue of a bipartite graph with multiplicity $m(\lambda)$, then so is $-\lambda$.
14.22. Show that a connected k-regular graph is bipartite if and only if $-k \in Sp(G)$. [Hint: Suppose $-k \in Sp(G)$ and that $(x_1 = 1, x_2, \ldots, x_n)^{\mathrm{T}}$ is an eigenvector corresponding to $-k$. Then if $v_{i_1}, \ldots, v_{i_k}$ are the neighbors of v_1, $x_{i_1} = x_{i_2} = \ldots = x_{i_k} = -1$. If v_j is a neighbor of v_{i_1}, $x_j = 1$, etc.]
14.23. Establish the inequality (11.16).
14.24. Prove: If $n \ge 5$, $L(K_n)$ is hyperenergetic.
14.25. Prove: If $n \ge 4$, $L(K_{n,n})$ is hyperenergetic.

Notes

Standard references for algebraic graph theory are [22, 47, 75].

Many variations of graph energy have been studied recently. Two types of energy of digraphs have been considered—skew energy of digraphs by taking the adjacency matrix of the digraph to be skew-symmetric [1, 171] and another by taking it to be the nonsymmetric $(0,1)$-matrix [157]. The Laplacian matrix of a simple graph G is the matrix $L = \Delta - A$, where Δ is the diagonal matrix whose diagonal entries are the degrees of the vertices of G, and A is the adjacency matrix of G. The energy of the matrix L is the Laplacian energy of G [85]. Yet another graph energy that has been studied is the distance energy of a graph [110]. It is the energy of the distance matrix $D = (d_{ij})$ of G, where d_{ij} is the distance between the vertices v_i and v_j of G. More generally, Nikiforov has introduced and studied [147] the concept of the energy of any p by q matrix.