Rooted Products, Tails

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See title.

1 Tails of Graphs

1.1 The Rooted Product

Assume we are given a graph X with $V(X) = \{1, \ldots, n\}$ and a sequence $\mathscr{Y}$ of rooted graphs $Y_1, \ldots, Y_n$, each with with at least one vertex. Let $X^{\mathscr{Y}}$ denote the graph obtained by merging the root of Y_r with the vertex r of X, for each r; we call it the *rooted product* of X with $\mathscr{Y}$.

Let $\mathscr{D}(t)$ denote the $n \times n$ diagonal matrix with rr-entry equal to $\phi(Y_r, t)$ and let $\mathscr{D}_1(t)$ be the $n \times n$ diagonal matrix with rr-entry equal to $\phi(Y_r \setminus r, t)$. The following result comes from [1]. 1

1.1 Theorem. *If X is a graph on n vertices with adjacency matrix A and $\mathscr{Y}$ is a sequence of n rooted graphs, then*

$$\phi(X^{\mathscr{Y}}, t) = \det(\mathscr{D}(t) - \mathscr{D}_1(t)A).$$

Proof. Let $\mathscr{Y}_1$ denote the sequence we get by replacing Y_1 with K_1, let $\psi = \phi(Y_1, t)$ and $\psi_1 = \phi(Y_1 \setminus 1, t)$. We set

$$M(X, \mathscr{F}) = D(\mathscr{Y}) - D_1(\mathscr{Y})A(X$$

(for any pair X and $\mathscr{Y}$). The first row of $D(\mathscr{Y}) - D_1(\mathscr{Y})A$ is equal to

$$(\psi - t\psi_1)e_1^T + \psi_1 e_1^T M(X, \mathscr{Y}_1).$$

If $\mathscr{Y}'$ denotes the sequence we get by deleting the first term from $\mathscr{Y}$, then by induction we have

$$\det(D(\mathscr{Y}) - D_1(\mathscr{Y})A) = (\psi - t\psi_1)\det(M(X \setminus 1, \mathscr{Y}')) + \psi_1 \det(M(X, \mathscr{Y}_1)).$$

Observe now that $X^{\mathscr{Y}}$ is the 1-sum of Y_1 and $X^{\mathscr{Y}_1}$, whence

$$\phi(X^{\mathscr{Y}}, t) = \phi(Y_1)\phi(X^{\mathscr{Y}_1}) + \phi(Y)\phi((X \setminus 1)^{\mathscr{Y}'}) - t\phi(Y_1)\phi((X \setminus 1)^{\mathscr{Y}'}).$$

On comparing these last two equations, the result follows. □

The graphs we will actually be concerned with are rooted products of some graph X with a collection of c copies of the path P_{n+1}. We use C to denote the vertices of X at which these paths are attached. We say that X is formed by attaching c tails to the vertices in the subset C of $V(X)$. Let $\varphi_n(t)$ denote $\phi(P_n, t)$.

1.2 Corollary. *Assume Z is obtained by adding c tails to X at the vertices in C. Let D be the diagonal matrix where $D_{u,u}$ is the number of tails on u. Then*

$$\phi(Z,t) = \phi(P_n,t)^c \det\left(tI - A - \frac{\varphi_{n-1}(t)}{\varphi_n(t)}D\right).$$

Right now the number of tails is 0 or 1. We will become more flexible.

Proof. From the theorem, we have

$$\phi(Z,t) = \phi(P_n,t)^c \det(\mathscr{D}_1(t)^{-1}\mathscr{D}(t) - A).$$

As

$$\varphi_{n+1}(t) = t\varphi_n(t) - \varphi_{n-1}(t),$$

we have

$$\frac{\varphi_{n+1}(t)}{\varphi_n(t)} = t - \frac{\varphi_{n-1}(t)}{\varphi_n(t)}$$

and the result follows. □

The rational function $t^{-1}\varphi_{n-1}(t^{-1})/\varphi_n(t^{-1})$ is the generating function for closed walks on P_n that start at vertex 1; its limit as $n \to \infty$ is the generating function for the Catalan numbers

1.2 Mutants

We may allow multiple tails on each vertex. In this case each vertex in C has a multiplicity, which will be a positive integer. If $u \in C$ we define $F_{u,u}$ to be the number of tails on u.

Let $Q_{r,n}$ denotes the graph formed when we merge the first vertices of r copies of P_n.

$Q_{r,n}$ is a subdivision of the star $K_{1,r}$

1.3 Lemma.

$$\phi(Q_{r,n},t) = \phi(P_{n-1},t)^{r-1}(t\phi(P_n,t) - r\phi(P_{n-1},t))$$

If $Q^1_{r,n}$ denote the graph we get by deleting the vertex of degree r, then

$$\frac{Q^1_{r,n}}{Q_{r,n}} = t - r\frac{\phi(P_{n-1},t)}{\phi(P_n,t)}.$$

It follows that, with our revised definition of F, Corollary 1.2 still holds.

2 Limits

2.1 Real Limits

We can write the recurrence for the characteristic polynomial of a path in matrix form:

$$\begin{pmatrix}\varphi_{n+1}\\ \varphi_n\end{pmatrix} = \begin{pmatrix}t & -1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\varphi_n\\ \varphi_{n-1}\end{pmatrix}, \qquad (n \ge 1) \tag{2.1}$$

whence

$$\begin{pmatrix}\varphi_{n+1}\\ \varphi_n\end{pmatrix} = \begin{pmatrix}t & -1\\ 1 & 0\end{pmatrix}^n\begin{pmatrix}t\\ 1\end{pmatrix}. \qquad (n \ge 0).$$

Set

$$M(t) = \begin{pmatrix} t & -1 \\ 1 & 0 \end{pmatrix}.$$

The eigenvalues of M are the roots of the quadratic

$$z^2 - tz + 1,$$

that is

$$\frac{1}{2}(t \pm \sqrt{t^2-4}).$$

We set

$$\alpha = \frac{1}{2}(t - \sqrt{t^2-4}),$$

and then the second root is α^{-1} and

$$t = \alpha + \alpha^{-1}.$$

If $t \neq 2$, the eigenvalues of $M(t)$ are distinct, and it follows that there are idempotent matrices F_0 and F_1 such that $F_0 + F_1 = I$ and

$$M(t)^n = \alpha^n F_0 + \alpha^{-n} F_1.$$

Therefore

$$\begin{pmatrix} \varphi_{n+1} \\ \varphi_n \end{pmatrix} = \alpha^n F_0 \begin{pmatrix} t \\ 1 \end{pmatrix} + \alpha^{-n} F_1 \begin{pmatrix} t \\ 1 \end{pmatrix}$$

2.1 Lemma. *If $t \in \mathbb{R}$ and $t > 2$, then*

$$\lim_{n\to\infty} \frac{\varphi_{n-1}(t)}{\varphi_n(t)} = \frac{1}{2}\big(t - \sqrt{t^2-4}\big);$$

if $t < 2$ we have

$$\lim_{n\to\infty} \frac{\varphi_{n-1}(t)}{\varphi_n(t)} = -\frac{1}{2}\big(t - \sqrt{t^2-4}\big);$$

Proof. If $|t| > 2$, then $\alpha^n \to 0$ as $n \to \infty$ and hence

$$\|M(t)^n - \alpha^{-n} F_0\| \to 0$$

as $n \to \infty$. Consequently

$$\begin{pmatrix} \varphi_{n-1}(t) \\ \varphi_n(t) \end{pmatrix} - \alpha^n F_0 \begin{pmatrix} t \\ 1 \end{pmatrix}$$

convergs to zero and this proves that

$$\lim_{n\to\infty} \frac{\varphi_{n-1}(t)}{\varphi_n(t)}$$

exists. From (2.1), we deduce that this limit must be an eigenvector for $M(t)$ with eigenvalue equal to the limit. As the eigenvalues of $M(t)$ are α and α^{-1}, our limit must be α. $\square$

$\varphi_{n-1}(t)/\varphi_n(t) < 1$ when n is large

We note that

$$M(t)\begin{pmatrix}\alpha\\1\end{pmatrix} = \begin{pmatrix}t\alpha-1\\ \alpha\end{pmatrix}$$

and $t\alpha - 1 = \alpha^2$, therefore

$$M(t)\begin{pmatrix}\alpha\\1\end{pmatrix} = \alpha\begin{pmatrix}\alpha\\1\end{pmatrix}.$$

2.2 Corollary. *If $t > 2$,*

$$\lim_{n\to\infty} tI - A - \frac{\varphi_{n-1}(t)}{\varphi_n(t)}F = tI - A - \frac{1}{2}\big(t - \sqrt{t^2-4}\big).$$ □

If we assume $\zeta = e^u$ and $t = \zeta + \zeta^{-1}$, then

$$tI - A - \frac{1}{2}\big(t - \sqrt{t^2-4}\big)F = (\zeta+\zeta^{-1})I - A - \zeta F.$$

What the scattering papers tell us is that, if ζ is complex with norm one and the columns of the $n \times c$ matrix P are the vectors e_r for r in C, then

$$S(\zeta) := (z - z^{-1})P^T((\zeta+\zeta^{-1})I - A - \zeta F)^{-1})P - I.$$

is unitary. In fact

$$S(\zeta)S(\zeta^{-1}) = I$$

for any value of ζ.

2.2 Some Complexity

If $t = 2\cos(\theta)$, the eigenvalues of

$$\begin{pmatrix}t & -1\\ 1 & 0\end{pmatrix}$$

are $e^{\pm i\theta}$, and then

$$\begin{pmatrix}t & -1\\ 1 & 0\end{pmatrix}^n\begin{pmatrix}t\\1\end{pmatrix} = e^{in\theta}F_0\begin{pmatrix}t\\1\end{pmatrix} + e^{-in\theta}F_1\begin{pmatrix}t\\1\end{pmatrix}.$$

Accordingly

$$\phi(P_n, 2\cos(\theta)) = Ae^{in\theta} + Be^{-in\theta}$$

for some scalars A and B (with $A + B = 1$). We see that $\varphi_{n-1}(t)/\varphi_n(t)$ does not converge in this case. We can still use Corollary 1.2 to compute the eigenvalues of the rooted product when the tails are finite, but we can say nothing intelligent about limits.

3 Graphs with Infinite Tails

3.1 Spectrum of an Infinite Graph

We restrict ourselves to graphs with an upper bound on their valency. If Z is a graph and f is a complex function on $V(Z)$, the *adjacency operator* A maps f to a function Af such that

$$(Af)(u) = \sum_{v\sim u} f(v).$$

The *spectrum* of A is the set of complex scalars λ such that $\lambda I - A$ is not invertible.

There are two ways in which $\lambda I - A$ might fail to be invertible:

(i) It might not be injective.

(ii) It might not be surjective.

When an operator acts on a finite dimensional space, it is injective if and only if it is surjective. By way of examples, if V is the space of real polynomials in t, multiplication by t is a linear map that is injective but not surjective; differentiation with respect to t is surjective but not injective.

We prefer that our linear operators act on Banach spaces, and there are three at hand. First is $\ell^\infty(Z)$, the space of bounded functions on Z. The second is $\ell^1(Z)$, the space of functions f such that

$$\sum_{v\in V(Z)} |f(v)| < \infty.$$

Finally we have $\ell^2(Z)$, consisting of the functions f such that

$$\sum_{v\in V} |f(v)|^2 < \infty.$$

We note that $\ell^\infty(Z)$ and $\ell^1(Z)$ are Banach spaces, while $\ell^2(Z)$ is a Hilbert space. In quantum physics, the operators of interest are usually defined only on a dense subspace of a Hilbert space. For example, consider differentiation acting on square-integrable functions on the interval $[0,1]$.

Now assume Z is formed by attaching infinite tails to vertices of a finite graph X. Functions in $\ell^2(Z)$ are known as *bound states*. An eigenvector with support contained in $V(X)$ is a *confined state* (a confined state is necessarily bound.) An eigenvector is a *scattering state* if it lies in $\ell^\infty(V(Z))\setminus \ell^2(V(Z))$.

3.2 Sequence Spaces

This section does not have much to do with scattering; it's more me reviewing my analysis

For our purposes, there are three sequence spaces of interest: $\ell^1(V(X))$, $\ell^2(V(X))$ and $\ell^\infty(V(X))$. These are Banach spaces (complete, normed) and $\ell^2(V(X))$ is a Hilbert space. We have the inclusions

$$\ell^1(V(X)) \subseteq \ell^2(V(X)) \subseteq \ell^\infty(V(X)).$$

The dual space of ℓ^1 is ℓ^∞, and vice versa (while ℓ^2 is self-dual).

If the valency of X is bounded, then its adjacency matrix A is bounded relative to all three norms. Scattering states lie in $\ell^\infty(V(X))$, but do not usually lie in ℓ^2. We use $\|\cdot\|_p$ to denote the ℓ^p-norm.

If $\mathscr{B}$ is a normed space and A is a linear operator on $\mathscr{B}$, the *operator norm* of A is

$$\sum_{\|x\|_{\mathscr{B}}=1} \|Ax\|_{\mathscr{B}}.$$

3.1 Lemma. *If X is finite then:*

(a) $\|A\|_1 = \max_i \|Ae_i\|_1$.

(b) $\|A\|_2 = \sigma_1$*, the largest singular value of A.*

(c) $\|A\|_\infty = \max_i \|e_i^T A\|_1$. □

We see that $\|A\|_\infty = \|A^T\|_1$. If $x \in \ell^1$ and $y \in \ell^\infty$, we define $\langle x, y\rangle$ by

$$\langle x, y\rangle = \sum_r x_r y_r.$$

Hölder's inequality gives us that

$$|\langle x, y\rangle| \le \|x\|_1 \|y\|_\infty;$$

It follows that we have a bilinear form on $\ell^1 \times \ell^\infty$.

If $x \in \ell^1$ and $y \in \ell^\infty$, define $L_{x,y}$ by

$$L_{x,y}(z) = \langle x, z\rangle\, y.$$

Then $L_{x,y}$ is a linear operator on ℓ^∞; it is idempotent if $\langle x, y\rangle = 1$.

3.3 Eigenvectors in $\ell^\infty(V(Z))$

An eigenvector z is *geometric* on a tail if $z_r = Ce^{ir\eta}$ for some positive scalar η. If X has c tails, $c \ge 2$, and $\theta = 2\cos(\eta)$, then an ℓ^∞-eigenvector is a *scattering state with incoming on the i-th tail* if it is geometric on all but the i-th tail. We will assume that on the i-th tail,

$$z_r = e^{-ir\eta} + \sigma_i e^{ir\eta}$$

and that on the j-th tail,

$$z_r = \sigma_j e^{ir\eta}.$$

3.2 Theorem. *Let Z be the rooted product of the graph X with c paths of infinite length. Let z be an eigenvector of Z in $\ell^\infty(V(Z))$ with eigenvalue θ and let $(z_r)_{r\ge 0}$ be the values of z on a tail. There are three cases:*

(a) $|\theta| < 2$*:* $\theta = 2\cos(\eta)$, $z_r = Ce^{ir\eta} + De^{-ir\eta}$*; the eigenvector is geometric if and only if* $z_1/z_0 = e^{i\eta}$.

(b) $|\theta| = 2$*: either* $\theta = 2$ *and* y_r *is constant, or* $\theta = -2$ *and* $z_r = C(-1)^r$ *for some real* γ*.*

(c) $|\theta| > 2$*:* $\theta = 2\cosh(\eta)$*,* $\eta > 0$*,* $z_r = z_0 e^{-r\eta}$*.*

Proof. We work from the expression

$$\begin{pmatrix} z_{r+1} \\ z_r \end{pmatrix} = S^r \begin{pmatrix} b \\ a \end{pmatrix}.$$

with

$$S = \begin{pmatrix} \theta & -1 \\ 1 & 0 \end{pmatrix}.$$

Set

$$\beta = \begin{pmatrix} b \\ a \end{pmatrix}.$$

Suppose $\theta = 2$. Then (simple induction)

$$S^n = \begin{pmatrix} n & 1-n \\ n-1 & 2-n \end{pmatrix}$$

and

$$S^n \begin{pmatrix} b \\ a \end{pmatrix} = \begin{pmatrix} n(b-a)+a \\ (n-1)(b-a)+a \end{pmatrix};$$

hence $S^n\beta$ is bounded if and only if $b = a$, and then z is constant. If $\theta = -2$, note that

$$\begin{pmatrix} -2 & -1 \\ 1 & 0 \end{pmatrix} = -\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 2 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

and then deduce that z is bounded if and only $a + b = 0$, in which case $z_r = c(-1^r)$ for some c.

Assume $|\theta| \neq 2$. Then the eigenvalues of S are distinct and their product is $\det(S)$, which is 1. There is a 2×2 idempotent F such that

$$S^r = \left(\frac{\theta + \sqrt{\theta^2 - 4}}{2}\right)^r F + \left(\frac{\theta - \sqrt{\theta^2 - 4}}{2}\right)^r (I - F)$$

If $|\theta| < 2$, both eigenvalues of S have absolute value 1, and therefore $S^r\beta$ is bounded.

As

$$S^r\beta = \begin{pmatrix} z_{r+1} \\ z_r \end{pmatrix},$$

we deduce that

$$\begin{pmatrix} z_{r+1} \\ z_r \end{pmatrix} = e^{ir\eta} F\beta - e^{-ir\eta}(I - F)\beta$$

and therefore z is geometric if and only if $(I - F)\beta = 0$, and this happens if and only if β is a eigenvector for S with eigenvalue $(\theta + \sqrt{\theta^2 - 4})/2$, i.e., with eigenvalue $e^{i\eta}$. To identify this eigenvector, note that

$$S\begin{pmatrix} e^{i\eta} \\ 1 \end{pmatrix} = \begin{pmatrix} (e^{i\eta} + e^{-i\eta})e^{i\eta} - 1 \\ e^{i\eta} \end{pmatrix} = e^{i\eta}\begin{pmatrix} e^{i\eta} \\ 1 \end{pmatrix}$$

If $|\theta| > 2$, then $(\theta + \sqrt{\theta^2 - 4})/2$ is greater than 1 and

$$S^m \beta$$

is unbounded unless $F\beta = 0$, which happens if and only if $(I - F)\beta = \beta$, that is, β is an eigenvector for S with eigenvalue of absolute value at most 1. Hence the eigenvector z is bounded if $|\theta| > 2$ and β is an eigenvector for S with eigenvalue

$$\mu = \frac{1}{2}(\theta - \sqrt{\theta^2 - 4}).$$

The adjugate of $S - \mu I$ is

$$R = \begin{pmatrix} -\mu & 1 \\ -1 & \theta - \mu \end{pmatrix}$$

and since

$$(S - \mu I)R = \det(S - \mu I)I = 0,$$

the columns of R are eigenvectors for S with eigenvalue μ. Therefore

$$\frac{b}{a} = \frac{1}{2}\big(\sqrt{\theta^2 - 4} - \theta\big). \qquad \square$$

In case (c), the vector z is a bound state.

3.3 Corollary. *An eigenvector z in $\ell^\infty(V(Z))$ with eigenvalue θ lies in ℓ_1 if and only if $|\theta| > 2$ or z is zero on C and on all tails.* $\square$

3.4 Another Quadratic

We show that

$$\zeta(\zeta + \zeta^{-1})I - A - \zeta F) = (I - \zeta A + \zeta^2 (I - F))$$

provides information about scattering states.

3.4 Theorem. *Let X be a graph with c tails, and let C be the set of vertices of attachment of the tails. Let z be a scattering state on X, incoming on the j-tail, with eigenvalue θ. Assume $\zeta = e^{i\theta}$ (so $\zeta + \zeta^{-1} = 2\cos(\theta)$). Let $z_{u,r}$ denote the value of z on vertex r of the tail attached to u in X, and let x denote the restriction of z to X. Let F be the diagonal matrix with $F_{u,u} = 1$ if $u \in C$ and $F_{u,u} = 0$ otherwise. Then $(I - \zeta A + \zeta^2 (I - F))x = (1 - \zeta^2)e_j$.*

Proof. Let $\theta = 2\cos(\eta)$ be the eigenvalue for z. If $u \in V(X) \setminus C$, then $x_u = z_{u,0}$. Hence, if $u \notin C$,

$$\theta x_u = \sum_{v \sim u, v \in X} x_v = (A(X)x)_u$$

and, if $u \in S$, then

$$\theta x_u = \sum_{v \sim u, v \in X} x_v + z_{u,1} = (A(X)x)_u + z_{u,1}.$$

We have $z_{u,1} = e^{i\eta} x_u$ if $u \neq i$; if $u = i$, then

$$z_{u,r} = \sigma_u e^{ir\eta} + e^{-i\eta r}.$$

Now

$$\theta z_{u,1} = z_{u,0} + z_{u,2}$$

and so

$$(e^{i\eta} + e^{-i\eta})(\sigma_u e^{i\eta} + e^{-i\eta}) = x_u + \sigma_u e^{2i\eta} + e^{-2i\eta},$$

yielding that $\sigma_u = x_u - 1$. Therefore

$$z_{u,1} = e^{i\eta} x_u - e^{i\eta} + e^{-i\eta}$$

Let R be the diagonal matrix with $R_{u,u} = 1$ if $u \in C$ and $R_{u,u} = 0$ otherwise. The above equations can be written as

$$\theta x = Ax + e^{i\eta} Rx - (e^{i\eta} - e^{-i\eta}) e_j.$$

Set $\zeta = e^{i\eta}$. Then

$$(\zeta + \zeta^{-1})x = Ax + \zeta Rx - (\zeta - \zeta^{-1}) e_j$$

and so

$$(-(\zeta + \zeta^{-1})I + \zeta R + A)x = (\zeta - \zeta^{-1}) e_j$$

and therefore

$$(I - \zeta A + \zeta^2 (I - R))x = (1 - \zeta^2) e_j. \qquad \square$$

If, for each j in C, the function $z(j)$ is a scattering state with incoming on tail j, then the set

$$\{z(j) : j \in S\}$$

is linearly independent—any linear combination of scattering states geometric on tail i is geometric on tail i, and so cannot be a scattering state with incoming on tail i.

3.5 Playing with Blocks

We develop some formulas for 2×2 Hermitian block matrices (with square diagonal blocks).

3.5 Lemma. *If C is invertible, the $(1,1)$-block of*

$$\begin{pmatrix} A & B^* \\ B & C \end{pmatrix}^{-1}$$

is equal to $(A - B^* C^{-1} B)^{-1}$.

Proof. We have the factorization

$$\begin{pmatrix} A & B^* \\ B & C \end{pmatrix} = \begin{pmatrix} I & 0 \\ 0 & C \end{pmatrix} \begin{pmatrix} I & B^* \\ 0 & 1 \end{pmatrix} \begin{pmatrix} A - B^* C^{-1} B & 0 \\ C^{-1} B & I \end{pmatrix}$$

and therefore

$$\begin{pmatrix} A & B^* \\ B & C \end{pmatrix}^{-1} = \begin{pmatrix} A - B^* C^{-1} B & 0 \\ C^{-1} B & I \end{pmatrix}^{-1} \begin{pmatrix} I & -B^* \\ 0 & 1 \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & C^{-1} \end{pmatrix},$$

from which our claim follows. □

The matrix $A - B^* C^{-1} B$ is the *Schur complement* of C. One consequence of the proof of the lemma is that

$$\det \begin{pmatrix} A & B^* \\ B & C \end{pmatrix} = \det(C) \det(A - B^* C^{-1} B).$$

3.6 Lemma. *Assume*

$$M = \begin{pmatrix} A & B^* \\ B & C \end{pmatrix}$$

and that the diagonal blocks of M are square. If

$$z = \begin{pmatrix} x \\ y \end{pmatrix}$$

is an eigenvector for M with eigenvalue λ and λ is not an eigenvalue of C, then

$$(\lambda I - A - B^* (\lambda I - C)^{-1} B) x = 0, \qquad y = (\lambda I - C)^{-1} B x.$$

Proof.

$$Mz = \begin{pmatrix} Ax + B^* y \\ Bx + Cy \end{pmatrix} = \begin{pmatrix} \lambda x \\ \lambda y \end{pmatrix}$$

yielding

$$B^* y = (\lambda I - A) x, \quad Bx = (\lambda I - C) y.$$

Hence

$$y = (\lambda I - C)^{-1} B x$$

and

$$(\lambda I - A) x = B^* y = B^* (\lambda I - C)^{-1} B x$$

and the lemma follows. □

We see from this lemma that if λ is an eigenvalue of M but not of C, then it is an eigenvalue of the Schur complement of C.

3.6 *The Scattering Matrix*

We apply the results on block matrices to $S(\zeta)$.

Let C be the first c vertices of X and let A_1 and A_2 respectively be the respective adjacency matrices of the subgraphs of X induced by C and $V(X)\setminus C$. Then

$$((\zeta+\zeta^{-1})I-A-\zeta D)^{-1}=\begin{pmatrix}(\zeta+\zeta^{-1})I-A_1-\zeta D & B^* \\ B & (\zeta+\zeta^{-1})I-A_2\end{pmatrix}^{-1}$$

We recall that if the columns of the $n\times c$ matrix P are the vectors $e_1,\dots,e_c$, then

$$S(\zeta):=(\zeta-\zeta^{-1})P^T\big((\zeta+\zeta^{-1})I-A-\zeta D)^{-1}\big)P-I.$$

Here $P^T((\zeta+\zeta^{-1})I-A-\zeta D)^{-1})P$ is the inverse of the Schur complement of the $(2,2)$-block of

$$\begin{pmatrix}(\zeta+\zeta^{-1})I-A_1-\zeta D & B^* \\ B & (\zeta+\zeta^{-1})I-A_2\end{pmatrix}.$$

We denote this complement by $Q(\zeta)$ and observe that

$$Q(\zeta)=(\zeta+\zeta^{-1})I-A-\zeta D-B^*((\zeta+\zeta^{-1})I-A_2)^{-1}B.$$

and accordingly

$$S(\zeta)=(\zeta-\zeta^{-1})Q(\zeta)^{-1}-I_c.$$

3.7 Lemma. *If $D=I_c$, then*

$$S(\zeta)S(\zeta^{-1})=I_c.$$

If in addition $|z|=1$, then $S(\zeta)$ is unitary.

Proof. We have

$$Q(\zeta)=(\zeta+\zeta^{-1})I_c-A-\zeta D-B^*\big((\zeta+\zeta^{-1})I-A_2\big)^{-1}B,$$

and so

$$Q(\zeta)-Q(\zeta^{-1})=(\zeta^{-1}-\zeta)D.$$

Hence

$$Q(\zeta^{-1})^{-1}Q(\zeta)-I_c=(\zeta^{-1}-\zeta)Q(\zeta^{-1})^{-1}D$$

and therefore

$$-Q(\zeta)^{-1}Q(\zeta^{-1})=(\zeta-\zeta^{-1})Q(z)^{-1}D-I_c.$$

If $D=I_c$, this yields

$$S(\zeta)=-Q(\zeta)^{-1}Q(\zeta^{-1}).$$

When $D=I_c$,

$$Q(\zeta)=\zeta^{-1}I_c-A-B^*((\zeta+\zeta^{-1})I_{n-c}-A_2)^{-1}B,$$

and

$$Q(\zeta^{-1}) = \zeta I_c - A - B^*((\zeta+\zeta^{-1})I - A_2)^{-1}B.$$

This implies that $Q(\zeta)$ and $Q(\zeta^{-1})$ commute, and this in turn implies that

$$S(\zeta)S(\zeta^{-1}) = Q(\zeta)^{-1}Q(\zeta^{-1})\,Q(\zeta^{-1})^{-1}Q(\zeta) = I_c$$

We conclude also that if $|z| = 1$, then $S(\zeta)$ is unitary. □

3.7 Reduced Walks

A walk in a graph X is *reduced* if it does not contain a subsequence of the form uvu. (The second and second-last vertices in a reduced closed walk of length greater than two might be the same.) If $|V(X)| = n$, then the matrix generating series $\Phi(X,t)$ is defined by declaring that $(\Phi(X,t))_{u,v}$ is the generating series for the reduced walks in X from u to v, for all vertices u and v of X. We see that if X is a tree, there is exactly one reduced walk between a given pair of vertices, and the length of the walk is the distance between the vertices. Hence if T is a tree, the entries of $\Phi(T,t)$ are polynomials of degree at most the diameter of T. Equivalently we can write

$$\Phi(T,t) = \sum_{r=0} t^r D_r,$$

where $(D_r)_{u,v} = 1$ if $\operatorname{dist}(u,v) = r$ and is otherwise zero. If T is a tree, then $\Phi'(T,1) = D(T)$.

If $A = A(X)$, define $p_r(A)$ to be the matrix (of the same order as A) such that $(p_r(A)_{u,v})$ is the number of reduced walks in X from u to v. Thus

$$\Phi(X,t) = \sum_r t^r p_r(A).$$

Observe that

$$p_0(A) = I, \quad p_1(A) = A, \quad p_2(A) = A^2 - \Delta,$$

where Δ is the diagonal matrix of valencies of X. If $r \geq 3$ we have the recurrence

$$Ap_r(A) = p_{r+1}(A) + \Delta_1 p_{r-1}(A).$$

These calculations were first carried out by Biggs, who observed the implication that $p_r(A)$ is a polynomial in A and Δ, of degree r in A.

We define Δ_1 to be $\Delta - I$. Our next theorem combines two results from Chan and Godsil [2]. 2

3.8 Theorem. *For any graph X on at least two vertices,*

$$\Phi(X,t)(I - tA + t^2\Delta_1) = (1-t^2)I.$$

Furthermore, $\det(I - tA + t^2\Delta_1) = 1 - t^2$ *if and only if T is a tree.*

Note that

$$(\zeta+\zeta^{-1})I - A - \zeta D)^{-1} = \zeta^{-1}(I - \zeta A - \zeta^2(D - I)).$$

The diffence in sign of the quadratic term (compared to that in the theorem) means we are unlikely to be able to relate the entries of $(I - \zeta A - \zeta^2(D - I))^{-1}$ to the numbers of some class of walks.