# ON THE MULTIPLICITY OF THE EIGENVALUES OF A GRAPH 

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#### Abstract

Given a graph $G$ with characteristic polynomial $\varphi(t)$, we consider the ML-decomposition $\varphi(t)=q_{1}(t) q_{2}(t)^{2} \ldots q_{m}(t)^{m}$, where each $q_{i}(t)$ is an integral polynomial and the roots of $\varphi(t)$ with multiplicity $j$ are exactly the roots of $q_{j}(t)$. We give an algorithm to construct the polynomials $q_{i}(t)$ and describe some relations of their coefficients with other combinatorial invariants of $G$. In particular, we get new bounds for the energy $E(G)=\sum_{i=1}^{n}\left|\lambda_{i}\right|$ of $G$, where $\lambda_{1}, \lambda_{2}, \ldots, \lambda_{n}$ are the eigenvalues of $G$ (with multiplicity). Most of the results are proved for the more general situation of a Hermitian matrix whose characteristic polynomial has integral coefficients.


## 1. Introduction

Let $A$ be a Hermitian $n \times n$ matrix such that the characteristic polyno$\operatorname{mial} \varphi_{A}(t)=\operatorname{det}\left(t I_{n}-A\right)$ has integral coefficients. We consider the multiplicity layered decomposition (ML-decomposition for short) of $\varphi_{A}(t)$ :

[^0]$(\mathrm{ML} 1) \varphi_{A}(t)=q_{1}(t) q_{2}(t)^{2} \ldots q_{m}(t)^{m}$ with $q_{j}(t) \in \mathbf{Z}[t]$ and $1 \neq q_{m}(t)$;
(ML2) $\lambda \in \mathbf{R}$ is a root of $\varphi_{A}(t)$ with multiplicity $j$ if and only if $q_{j}(\lambda)=0$.

Obviously, if $\varphi_{A}(t)$ has no roots of multiplicity $j$, then $q_{j}(t)=1$. We shall give an algorithmic construction of the polynomials $q_{j}(t)$ using the Euclidean algorithm in the family of derivatives $\varphi_{A}^{(j)}(t)$ of $\varphi_{A}(t)$. We show that the following properties are satisfied by the ML-decomposition.
(ML3) $\lambda$ is a root of $q_{j}(t)$ if and only if for every principal $i \times i$ submatrix $B$ of $A$ with $n-j+1 \leqq i \leqq n$, we have $\varphi_{B}(\lambda)=0$ and $\varphi_{B^{\prime}}(\lambda) \neq 0$ for a principal $(n-j) \times(n-j)$ submatrix $B^{\prime}$ of $A$.
(ML4) For $1 \leqq j \leqq m-1$ the derivative $\varphi_{A}^{(j)}(t)$ accepts an ML-decomposition $\varphi_{A}^{(j)}(t)=\hat{q}_{j+1}(t) q_{j+2}(t)^{2} \ldots q_{m}(t)^{m-j}$ with $\hat{q}_{j+1}(t)=r_{j}(t) q_{j+1}(t)$ for some $r_{j}(t) \in \mathbf{Z}[t]$, such that the simple roots of $\varphi_{A}^{(j)}(t)$ are exactly the roots of $\hat{q}_{j+1}(t)$.

Motivation for considering the ML-decomposition arises from applications to connected graphs $G$ without loops or multiple edges and its characteristic polynomial $\varphi_{G}(t)=\varphi_{A(G)}(t)$ where $A(G)$ is the adjacency matrix of $G$. Multiplicities of roots of $\varphi_{G}(t)$ are related to symmetries of the graph $G[3$, Ch. 6], regularity properties [3, Ch. 7] and important structural properties of the graph $G$. Moreover, in this paper we get further elementary applications of the ML-decomposition for $\varphi_{G}(t)$. Indeed, let $q_{j}(t)=t^{n_{j}}+a_{j 1} t^{n_{j-1}}+\cdots$ $+a_{j n_{j}}$ be the polynomials obtained from the ML-decomposition. We show the following:
(a) $\varphi_{G}(t)=q_{1}(t) q_{2}(t)^{2} \ldots q_{m}(t)^{m}$ with $m=m(G)$ maximal $j$ such that $n_{j} \geqq 1$.
(b) $n_{1} \geqq 1$, since the spectral radius $\rho(G)=\max \left\{\|\lambda\|: \varphi_{G}(\lambda)=0\right\}$ is a simple root of $\varphi_{G}(t)$.
(c) If $K=G \backslash\left\{a_{1}, \ldots, a_{k}\right\}$ is obtained from $G$ by deleting the vertices $a_{1}, \ldots, a_{k}$, then $m(G) \leqq m(K)+k$.
(d) $\frac{\varphi_{G}^{\prime}(t)}{\varphi_{G}(t)}=\sum_{j=1}^{m} j \frac{q_{j}^{\prime}(t)}{q_{j}(t)}$; which implies that a real number $\lambda$ is a root of $\varphi_{G}(t)$ with multiplicity $m_{\lambda}$ if and only if $\lim _{t \rightarrow \lambda} \frac{(t-\lambda) \varphi_{G}^{\prime}(t)}{\varphi_{G}(t)}=m_{\lambda}$.
(e) The minimal polynomial of $A(G)$ is $\mu_{G}(t)=q_{1}(t) q_{2}(t) \ldots q_{m}(t)$. In particular, $\sum_{j=1}^{m} n_{j} \geqq \operatorname{diam}(G)+1$, where $\operatorname{diam}(G)$ is the diameter of the graph $G$. As a consequence we also get $m(G) \leqq n-\operatorname{diam}(G)$.

For any polynomial $q(t)$ with real roots, define the energy of $q(t)$ by $E(q(t))=\sum|\lambda|$, where $\lambda$ runs over the roots of $q(t)$, counting multiplicities.
(f) $E(G)=\sum_{j=1}^{m} j E\left(q_{j}(t)\right)$, which yields the following McClelland-type bounds for the energy:

$$
\sum_{j=1}^{m} j \sqrt{a_{j 1}^{2}-2 a_{j 2}+n_{j}\left(n_{j}-1\right)\left|a_{j n_{j}}\right|^{2 / n_{j}}} \leqq E(G) \leqq \sum_{j=1}^{m} j \sqrt{n_{j}\left(a_{j 1}^{2}-2 a_{j 2}\right)}
$$

## 2. The multiplicity layered decomposition

2.1. Let $A$ be a Hermitian $n \times n$ matrix such that the characteristic polynomial $\varphi_{A}(t)$ has integral coefficients. Then the eigenvalues of $A$ are the roots of $\varphi_{A}(t)$, all of them real $\lambda_{1} \leqq \lambda_{2} \leqq \cdots \leqq \lambda_{n}$. For any eigenvalue $\lambda$ of $A$, we denote by $m_{\lambda}$ the multiplicity of $\lambda$ (writing $m(A, \lambda)$ if some confusion arises).

We shall consider irreducible polynomials in $\mathbf{Z}[t]$ (or equivalently in $\mathbf{Q}[t]$ ).
Lemma. Let $\lambda$ be an eigenvalue of $A$ with multiplicity $m_{\lambda}$. Let $q(t)$ be an irreducible polynomial such that $q(\lambda)=0$. Then the following happen:
(a) $q(t)$ has minimal degree among those polynomials $p(t) \in \mathbf{Z}[t]$ with $p(\lambda)=0$.
(b) If $q\left(\lambda^{\prime}\right)=0$ for some $\lambda^{\prime} \in \mathbf{C}$, then $\lambda^{\prime}$ is an eigenvalue of $A$ with $m_{\lambda^{\prime}}=m_{\lambda}$.

Proof. (a) In fact $q(t)$ generates the ideal in $\mathbf{Z}[t]$ of those $p(t)$ with $p(\lambda)=0$.
(b) $q(t)$ divides $\varphi_{A}(t)$, hence $\lambda^{\prime}$ is an eigenvalue of $A$. The multiplicity $m_{\lambda}$ is the maximal $i$ such that $q(t)^{i}$ divides $\varphi_{A}(t)$. Therefore $m_{\lambda}=m_{\lambda^{\prime}}$.
2.2. According to (2.1) we consider irreducible polynomials $p_{1}(t), \ldots$, $p_{s}(t) \in \mathbf{Z}[t]$ such that each $\lambda_{i}$ is a root of exactly one $p_{j}(t), 1 \leqq i \leqq n$. For each $1 \leqq i \leqq s$, consider $r(j)=\max \left\{k: p_{j}(t)^{k}\right.$ divides $\left.\varphi_{A}(t)\right\}$. Set

$$
q_{i}(t)=\prod_{r(j)=i} p_{j}(t)
$$

which yields an ML-decomposition $\varphi_{A}(t)=q_{1}(t) q_{2}(t)^{2} \ldots q_{m}(t)^{m}$.
Since $\varphi_{A}(t)$ is a monic polynomial, we may assume that each $p_{j}(t)$ and also $q_{j}(t)$ are monic polynomials. Set $m(G)=\max \left\{j: q_{j}(t) \neq 1\right\}$. We shall need the following:

Lemma (cf. [1]). $\varphi_{A}^{(k)}(t)=k!\sum_{\mathcal{P}_{n-k}(A)} \varphi_{B}(t)$, where the sum runs over the set $\mathcal{P}_{n-k}(A)$ of all principal $(n-k) \times(n-k)$-submatrices of $A$.

Proof. The proof in [1] considers the case $k=1$. The general statement follows by induction.
2.3. Proposition. For a root $\lambda$ of $\varphi_{A}(t)$ the following are equivalent:
(a) $\lambda$ has multiplicity $k$.
(b) $q_{k}(\lambda)=0$.
(c) For any principal $j \times j$-submatrix $B$ of $A$ with $n-k+1 \leqq j \leqq n$, we have $\varphi_{B}(\lambda)=0$ and $\varphi_{B^{\prime}}(\lambda) \neq 0$ for some $(n-k) \times(n-k)$-submatrix $B^{\prime}$ of $A$.

Proof. (a) $\Leftrightarrow(\mathrm{b})$ is clear.
(b) $\Rightarrow(\mathrm{c})$ Let $\lambda_{1} \leqq \lambda_{2} \leqq \cdots \leqq \lambda_{n}$ be the eigenvalues of $A$ and $\mu_{1} \leqq \mu_{2}$ $\leqq \cdots \leqq \mu_{j}$ those of a principal $j \times j$-submatrix $B$ of $A$ with $n-k+1 \leqq j \leqq n$, then by the interlacing theorem (see for example [3] for other applications):

$$
\lambda_{i} \leqq \mu_{i} \leqq \lambda_{n-j+i}, \quad(i=1, \ldots, j)
$$

If $\lambda_{t}=\lambda_{t+1}=\cdots=\lambda_{t+k-1}=\lambda$, then $\lambda_{t} \leqq \mu_{t} \leqq \lambda_{n-j+t}$ with $n-j+t \leqq t+$ $k-1$ and $\mu_{t}=\lambda$.

In case $\lambda$ is a root of all $B \in \mathcal{P}_{k}(A)$, then by the lemma above, $\varphi_{A}^{n-k}(\lambda)$ $=0$ and $\lambda$ has multiplicity at least $k+1$, a contradiction.
(c) $\Rightarrow$ (a) Apply again the Lemma.
2.4. Let $A$ be a Hermitian matrix with characteristic polynomial $\varphi_{A}(t)$ $\in \mathbf{Z}[t]$. Let $\varphi_{A}(t)=\prod_{j=1}^{m} q_{i}(t)^{i}$ the ML-decomposition with $q_{m}(t) \neq 1$.

LEMMA. $q_{m}(t)=\operatorname{mcd}\left(\varphi_{A}(t), \varphi_{A}^{(1)}(t), \ldots, \varphi_{A}^{(m-1)}(t)\right)$.
Proof. The claim follows from a straightforward but tedious calculation, we shall illustrate only the case $m=3$.

$$
\begin{gathered}
\varphi_{A}=q_{1} q_{2}^{2} q_{3}^{3}(\text { omitting the variable } t) \\
\varphi_{A}^{\prime}=q_{1}^{\prime} q_{2}^{2} q_{3}^{3}+2 q_{1} q_{2} q_{2}^{\prime} q_{3}^{3}+3 q_{1} q_{2}^{2} q_{3}^{2} q_{3}^{\prime}=\left(q_{1}^{\prime} q_{2} q_{3}+2 q_{1} q_{2}^{\prime} q_{3}+3 q_{1} q_{2} q_{3}^{\prime}\right) q_{2} q_{3}^{2}
\end{gathered}
$$

where the polynomial $r_{1}$ in parenthesis is not divisible by any $q_{i}, i=1,2,3$. (Indeed, if $p$ is an irreducible factor of $q_{1}$ dividing also $r_{1}$, then $p \mid q_{1}^{\prime} q_{2} q_{3}$. By (2.1), $p \nmid q_{i}, i=2,3$ and therefore $p \mid q_{1}^{\prime}=p^{\prime} s+p s^{\prime}$ where $s \in \mathbf{Z}[t]$ such that $q_{1}=p s$. This implies $p \mid p^{\prime} s$ and $p \mid s$, which in turn implies that $q_{1}$ has multiple roots, a contradiction. The cases $i=2,3$ are similar.) Now, $\varphi_{A}^{\prime \prime}=$ $r_{2} q_{3}$ with $r_{2}=r_{1}^{\prime} q_{2} q_{3}+r_{1} q_{2}^{\prime} q_{3}+2 r_{1} q_{2} q_{3}^{\prime}$ is not divisible by any $q_{i}, i=1,2,3$. Hence $q_{3}=\operatorname{mcd}\left(\varphi_{A}, \varphi_{A}^{\prime}, \varphi_{A}^{\prime \prime}\right)$.

The inductive construction of the polynomials $q_{1}(t), \ldots, q_{m}(t)$ is easily carried out:

$$
\begin{gathered}
q_{m}(t)=\operatorname{mcd}\left(\varphi_{A}(t), \varphi_{A}^{\prime}(t), \ldots, \varphi_{A}^{(m-1)}(t)\right) \\
q_{m-1}(t)=\operatorname{mcd}\left(\frac{\varphi_{A}(t)}{q_{m}(t)^{m}}, \frac{\varphi_{A}^{\prime}(t)}{q_{m}(t)^{m-1}}, \ldots, \frac{\varphi_{A}^{(m-2)}(t)}{q_{m}(t)^{2}}\right), \\
\vdots \\
q_{2}(t)=\operatorname{mcd}\left(\frac{\varphi_{A}(t)}{q_{3}(t)^{3} \ldots q_{m}(t)^{m}}, \frac{\varphi_{A}^{\prime}(t)}{q_{3}(t)^{2} \ldots q_{m}(t)^{m-1}}\right), \\
q_{1}(t)=\frac{\varphi_{A}(t)}{q_{2}(t)^{2} q_{3}(t)^{3} \ldots q_{m}(t)^{m}}
\end{gathered}
$$

2.5. To get more precise information on the derivatives of $\varphi_{A}(t)$ we need some results of elementary analysis.

Proposition. Let $p(t)$ be a polynomial of degree $n$ whose roots are real. Then the following hold:
(a) For every $1 \leqq j \leqq n-1$, $p^{(j)}(t)$ has only real roots.
(b) If $\lambda_{1} \leqq \lambda_{2} \leqq \cdots \leqq \lambda_{n}$ are the roots of $p(t)$ and $\mu_{1} \leqq \mu_{2} \leqq \cdots \leqq \mu_{j}$ the roots of $p^{(j)}(t)$, then $\lambda_{i} \leqq \mu_{i} \leqq \lambda_{n-j+i}(i=1, \ldots, j)$.
2.6. Let $\varphi_{A}(t)=\prod_{i=1}^{m} q_{i}(t)^{i}$ be the ML-decomposition as above.

Proposition. For any $i \geqq 1$, the following is an $M L$-decomposition:

$$
\varphi_{A}^{(i)}(t)=\left(r_{i}(t) q_{i+1}(t)\right) q_{i+2}(t)^{2} \ldots q_{m}(t)^{m-i}
$$

that is, $\lambda$ is a simple root of $\varphi_{A}^{(i)}(t)$ if and only if $r_{i}(\lambda)=0$ or $q_{i+1}(\lambda)=0$, where $r_{i}=r_{i-1}^{\prime} q_{i} q_{i+1} \ldots q_{m}+\sum_{j=0}^{m-i}(j+1) r_{i-1} q_{i} \ldots q_{i+j-1} q_{i+j}^{\prime} q_{i+j+1} \ldots q_{m}$, with $r_{0}(t)=1$.

Proof. The given decomposition follows by induction. It is enough to show that $\lambda$ is a simple root of $\varphi_{A}^{(i)}(t)$ if and only if $r_{i}(\lambda)=0$ or $q_{i+1}(\lambda)=0$. We show it by induction on $i$, the case $i=0$ being clear.

Assume $q_{i+1}(\lambda)=0$ and $\lambda$ is not a simple root of $\varphi_{A}^{(i)}(t)$. Then by (2.1), $r_{i}(\lambda)=0$. Hence $r_{i-1}(\lambda) q_{i}(\lambda) q_{i+1}^{\prime}(\lambda) q_{i+1}(\lambda) \ldots q_{m}(\lambda)=0$ and only $r_{i-1}(\lambda)$ $=0$ is possible, which contradicts the induction hypothesis.

Assume $r_{i}(\lambda)=0$ and $\lambda$ is not a simple root of $\varphi_{A}^{(i)}(t)$. By (2.5), $\lambda$ is also a root of $\varphi_{A}^{(i-1)}(t)=\left(r_{i-1}(t) q_{i}(t)\right) q_{i+1}(t)^{2} \ldots q_{m}(t)^{m-i+1}$.

If $r_{i-1}(\lambda)=0$, by induction hypothesis, $\lambda$ is a simple root of $\varphi_{A}^{(i-1)}(t)$. On the other hand, $r_{i-1}^{\prime}(\lambda) q_{i}(\lambda) \ldots q_{m}(\lambda)=0$ and either $r_{i-1}^{\prime}(\lambda)=0$ or $q_{i+j}(\lambda)$ $=0$ (for any $0 \leqq j \leqq m-i$ ) yield a contradiction.

If $q_{i+j}(\lambda)=0$ for some $0 \leqq j \leqq m-i$, we get

$$
r_{i-1}(\lambda) q_{i}(\lambda) \ldots q_{i+j-1}(\lambda) q_{i+j}^{\prime}(\lambda) \ldots q_{m}(\lambda)=0
$$

which also yields a contradiction.
The converse of the claim is clear.
2.7. The following result shows an interesting relation between the polynomials $r_{i}(t)$ as defined in (2.6).

Proposition. For $1 \leqq i \leqq m-1$, and for any $\lambda \in \mathbf{R}$, we have

$$
r_{i}(\lambda)^{2} \geqq r_{i-1}(\lambda) q_{i}(\lambda) r_{i+1}(\lambda) .
$$

Proof. Any polynomial $p(t)$ having only real roots $\mu_{1} \leqq \mu_{2} \leqq \cdots \leqq \mu_{n}$ satisfies

$$
\frac{p^{\prime}(t)}{p(t)}=\sum_{i=1}^{n} \frac{1}{t-\mu_{i}} \quad \text { and } \quad \frac{p^{\prime \prime}(t) p(t)-p^{\prime}(t)^{2}}{p(t)^{2}}=-\sum_{i=1}^{n} \frac{1}{\left(t-\mu_{i}\right)^{2}}
$$

which is negative for any $\lambda \neq \mu_{i}(1 \leqq i \leqq n)$. Hence

$$
p^{\prime}(\lambda)^{2} \geqq p^{\prime \prime}(\lambda) p(\lambda) \quad \text { for any } \quad \lambda \in \mathbf{R} .
$$

Applying this inequality for $p(t)=\varphi_{A}^{(i)}(t)$ and using (2.6) the result follows.

## 3. ML-decomposition for graphs

3.1. Let $G$ be a connected graph without loops or multiple edges. Let $1, \ldots, n$ be the vertices of $G$ and $A=A(G)$ its adjacency matrix. The results of Section 2 apply since $A$ is a symmetric matrix and the characteristic polynomial $\varphi_{G}(t)$ has integral coefficients. Set $\varphi_{G}(t)=t^{n}+a_{1} t^{n-1}+\cdots+a_{n}$ and let $\lambda_{1} \leqq \lambda_{2} \leqq \cdots \leqq \lambda_{n}$ be its (real) roots.

Consider the ML-decomposition $\varphi_{G}(t)=\prod_{j=1}^{m} q_{j}(t)^{j}$ with $n_{m} \geqq 1$, where $n_{j}$ is the degree of $q_{j}(t)$ (write $m(G):=m$ ). The Perron-Frobenius Theorem (see [4]) says that the spectral radius $\rho(G)$ is a simple root of $\varphi_{G}(t)$. Therefore $q_{1}(t) \neq 1$.

The minimal polynomial is $\mu_{G}(t)=\prod_{j=1}^{m} q_{j}(t)$.
3.2. Examples. (1) Let $G$ be the cubic graph

with 10 vertices and characteristic polynomial

$$
\varphi(t)=t^{10}-15 t^{8}-4 t^{7}+75 t^{6}+24 t^{5}-157 t^{4}-36 t^{3}+144 t^{2}+16 t-48
$$

Then

$$
\begin{aligned}
& q_{1}(t)=t^{2}-5 t+6=(t-3)(t-2) \quad \text { and } \quad \rho(G)=3, \\
& q_{2}(t)=t+1, \quad q_{3}(t)=t^{2}+t-2=(t-1)(t+2) .
\end{aligned}
$$

The ML-decompositions of the derivatives of $\varphi(t)$ are as follows:

$$
\begin{gathered}
\varphi^{\prime}(t)=\left[\left(5 t^{4}-15 t^{3}-10 t^{2}+36 t+2\right)(t+1)\right][(t-1)(t+2)]^{2} \\
\varphi^{\prime \prime}(t)=\left[\left(15 t^{6}-15 t^{5}-95 t^{4}+37 t^{3}+148 t^{2}+6 t-24\right)(t-1)(t+2)\right] .
\end{gathered}
$$

(2) Let $G$ be the cubic graph

with 12 vertices and with characteristic polynomial

$$
\begin{gathered}
\varphi(t)=t^{12}-18 t^{10}-2 t^{9}+117 t^{8}+72 t^{7}-339 t^{6} \\
-306 t^{5}+414 t^{4}+532 t^{3}-99 t^{2}-324 t-108
\end{gathered}
$$

Then

$$
\begin{gathered}
q_{1}(t)=t-3 \quad \text { and } \quad \rho(G)=3 \\
q_{2}(t)=t^{3}-t^{2}-5 t+6=(t-2)\left(t^{2}+t-3\right) \quad \text { with roots } \quad-2.3<1.3<2 \\
q_{5}(t)=t+1
\end{gathered}
$$

3.3. Let $G$ be a graph as in (3.1). The principal $(n-k) \times(n-k)$ submatrices of $A(G)$ correspond to the full subgraphs of $G$ obtained by deleting $k$ vertices. Then (2.2) and (2.3) yield:

Proposition. Let $\lambda$ be a root of $\varphi_{G}(t)$. The following are equivalent:
(a) $\lambda$ has multiplicity $k$.
(b) $q_{k}(\lambda)=0$.
(c) For any full subgraph $K=G \backslash\left\{a_{1}, \ldots, a_{j}\right\}$ with $n-k+1 \leqq j \leqq n$ we have $\varphi_{K}(\lambda)=0$ and there is a full subgraph $K^{\prime}=G \backslash\left\{a_{1}, \ldots, a_{n-k}\right\}$ with $\varphi_{K^{\prime}}(\lambda) \neq 0$.

Corollary. Let $K=G \backslash\left\{a_{1}, \ldots, a_{k}\right\}$ be a full subgraph of $G$. Then $m(G) \leqq m(K)+k$.
3.4. For any polynomial $p(t)$ with (possibly repeated) real roots $\lambda_{1} \leqq \lambda_{2}$ $\leqq \cdots \leqq \lambda_{n}$, we have

$$
\frac{p^{\prime}(t)}{p(t)}=\sum_{i=1}^{n} \frac{1}{t-\lambda_{i}}
$$

Hence for the ML-decomposition we get

$$
\frac{\varphi_{G}^{\prime}(t)}{\varphi_{G}(t)}=\sum_{j=1}^{m} j \frac{q_{j}^{\prime}(t)}{q_{j}(t)}
$$

There are several uses of these rational functions (see [5, Ch. 2]). Two important facts are the following:
(a) $\lim _{t \rightarrow \lambda} \frac{\varphi_{G}^{\prime}(t)(t-\lambda)}{\varphi_{G}(t)}=m_{\lambda}$ is the multiplicity of $\lambda$ as a root of $\varphi_{G}(t)$.
(b) $\frac{\varphi_{G}^{\prime}(t)}{\varphi_{G}(t)}=\sum_{r \geqq 0} \operatorname{tr}\left(A(G)^{r}\right) x^{-(r+1)}$ is the generating function in the variable $x^{-1}$.

Note that $\operatorname{tr}\left(A(G)^{r}\right)$ counts the number of closed walks of length $r$ in $G$.

For the polynomials $q_{j}(t)=t^{n_{j}}+a_{j 1} t^{n_{j}-1}+\cdots+a_{j n_{j}}$ we define the companion matrix

$$
A_{j}=\left[\begin{array}{ccccc}
-a_{j 1} & -a_{j 2} & \ldots & -a_{j n_{j-1}} & -a_{j n_{j}} \\
1 & 0 & \ldots & 0 & 0 \\
0 & 1 & \ldots & 0 & 0 \\
& & \ddots & \vdots & \vdots \\
& 0 & & & 1
\end{array}\right]
$$

which satisfies $\operatorname{det}\left(t I_{n_{j}}-A_{j}\right)=q_{j}(t)$. The trace of the powers $A_{j}^{r}$ is easily written as a polynomial in the coefficients $a_{j 1}, \ldots, a_{j n_{j}}$. For instance:

$$
\operatorname{tr}\left(A_{j}\right)=-a_{j 1}, \quad \operatorname{tr}\left(A_{j}^{2}\right)=a_{j 1}^{2}-2 a_{j 2}, \quad \operatorname{tr}\left(A_{j}^{3}\right)=-a_{j 1}^{3}+3 a_{j 1} a_{j 2}-2 a_{j 3} .
$$

Proposition. $\operatorname{tr}\left(A(G)^{r}\right)=\sum_{j=1}^{m} j \operatorname{tr}\left(A_{j}^{r}\right)$.
3.5. The diameter $\operatorname{diam}(G)$ of $G$ is the longest distance between two vertices of $G$.

Proposition. (a) $\sum_{j=1}^{m(G)} n_{j} \geqq \operatorname{diam}(G)+1$.
(b) $\sum_{j=2}^{m(G)}(j-1) n_{j} \leqq n-\operatorname{diam}(G)-1$.
(c) $m(G) \leqq n-\operatorname{diam}(G)$.

Proof. (a) $\sum_{j=1}^{m(G)} n_{j}$ is the number of distinct eigenvalues of $G$. This number is at least $\operatorname{diam}(G)+1$ (see for example $[3,3.13]$ ).
(b) Since $n=\sum_{j=1}^{m(G)} j n_{j}$, the inequality follows from (a).
(c) Follows from (b).

## 4. The energy of a graph and the ML-decomposition

4.1. The purpose of this section is to obtain McClelland-type bounds for the energy of a graph as an application of the ML-decomposition.

First observe that McClelland's bounds hold for quite general situations namely:

Theorem (cf. [7]). Let $A$ be a Hermitian $n \times n$-matrix and let $E(A)$ $=\sum_{i=1}^{n}\left|\lambda_{i}\right|$ be the energy of $A$, where $\lambda_{1} \leqq \lambda_{2} \leqq \cdots \leqq \lambda_{n}$ are the eigenvalues of $A$ counted with multiplicities. Then

$$
\sqrt{\operatorname{tr}\left(A^{2}\right)+n(n-1)|\operatorname{det} A|^{2 / n}} \leqq E(A) \leqq \sqrt{n \operatorname{tr}\left(A^{2}\right)}
$$

Proof (cf. [6]). We have

$$
E(A)^{2}=\sum_{i=1}^{n}\left|\lambda_{i}\right|^{2}+2 \sum_{j<k}\left|\lambda_{j}\right|\left|\lambda_{k}\right|=\operatorname{tr}\left(A^{2}\right)+n(n-1) \operatorname{AM}\left\{\left|\lambda_{j}\right|\left|\lambda_{k}\right|\right\},
$$

where AM denotes the arithmetic mean. Let GM $\left\{\left|\lambda_{j}\right|\left|\lambda_{k}\right|\right\}=|\operatorname{det} A|^{2 / n}$ be the geometric mean. Then $\mathrm{GM} \leqq \mathrm{AM}$ yields the first inequality.

Moreover, the variance of the numbers $\left|\lambda_{j}\right|, j=1,2, \ldots, n$ is:

$$
\begin{gathered}
0 \leqq \operatorname{var}\left\{\left|\lambda_{j}\right|\right\}=\operatorname{AM}\left\{\left|\lambda_{j}\right|^{2}\right\}-\left(\operatorname{AM}\left\{\left|\lambda_{j}\right|\right\}\right)^{2} \\
=\frac{1}{n} \sum_{j=1}^{n}\left|\lambda_{j}\right|^{2}-\left[\frac{1}{n} \sum_{j=1}^{n}\left|\lambda_{j}\right|\right]^{2}=\frac{1}{n} \operatorname{tr}\left(A^{2}\right)-\left(\frac{E(A)}{n}\right)^{2}
\end{gathered}
$$

and the second inequality holds.
4.2. Theorem. We have

$$
\sum_{j=1}^{m(G)} j \sqrt{\left[a_{j 1}^{2}-2 a_{j 2}\right]+n_{j}\left(n_{j}-1\right)\left|a_{j n_{j}}\right|^{2 / n_{j}}} \leqq E(G) \leqq \sum_{j=1}^{m(G)} j \sqrt{n_{j}\left[a_{j 1}^{2}-2 a_{j 2}\right]} .
$$

Proof. Using that

$$
\frac{\varphi_{G}^{\prime}(t)}{\varphi_{G}(t)}=\sum_{j=1}^{m(G)} j \frac{q_{j}^{\prime}(t)}{q_{j}(t)} \quad \text { and } \quad n=\sum_{j=1}^{m(G)} j n_{j},
$$

and Coulson Theorem [2], we get

$$
\begin{gathered}
E(G)=\frac{1}{\pi} \int_{-\infty}^{\infty}\left[n-\frac{i t \varphi_{G}^{\prime}(i t)}{\varphi_{G}(i t)}\right] d t=\sum_{j=1}^{m(G)} \frac{j}{\pi} \int_{-\infty}^{\infty}\left[n_{j}-\frac{i t q_{j}^{\prime}(i t)}{q_{j}(i t)}\right] d t \\
=\sum_{j=1}^{m(G)} j E\left(A_{j}\right),
\end{gathered}
$$

where $A_{j}$ is the companion matrix of $q_{j}(t)$. Here $i=\sqrt{-1}$.
By (3.4), $\operatorname{tr}\left(A_{j}^{2}\right)=a_{j 1}^{2}-2 a_{j 2}$ and $\operatorname{det} A_{j}=a_{j n_{j}}$. The result follows from (4.1).
4.3. As an example we calculate McClelland bounds and the bounds (4.2) for the graph (3.2 (2)):

| McClelland's bounds | lower | $E(G)$ | upper |
| :---: | :---: | :---: | :---: |
|  | 17.94 |  | 20.19 |
|  |  | 19.2 |  |
| (4.2) bounds | 19.1 |  | 19.48 |

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[^0]:    *This work was done during a visit of the second named author to UNAM.
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